CERN summer student work project report:
Data Taking and Simulation-Based Data Analysis at the ASACUSA Experiment

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A series of measurements and fine-tunings as well as the development of a new fit routine has been developed for the hydrogen beam of ASACUSA in preparation for the antihydrogen experiment. The B-field amplitude of the microwave cavity of the hydrogen beamline has been maximized, and the cavity characterized with careful measurements at various frequencies and amplitudes. The new fit routine performs cubic spline interpolation of simulated data in order to generate fit functions. Since the simulated data are numerical solutions of the theoretical equations that describe the system, such fit functions are better suited than the previously used ones. By using the settings found to be optimal, a set of measurements of the Rabi oscillations of hydrogen atoms have been performed, which, when fitted with the new routine, yields a value of (1 420 405 756.9 ± 9.1) Hz for the hyperfine transition frequency.

INTRODUCTION

This report describes the work carried out, the methods employed, and the results achieved over a 10-weeks internship at CERN as part of their summer student program. The internship lasted from June 23 to August 30, 2014, and took place in collaboration with the hydrogen beam section of the ASACUSA experiment, the ultimate goal of which is to perform spectroscopy on antihydrogen as a test of CPT symmetry.

The hyperfine structure is a consequence of the coupling of the total angular momentum of the proton to the total angular momentum of the orbital electron. The coupling results in the ground state splitting into four states: one triplet ($F = 1$, $M = -1, 0, 1$) and one singlet ($F = 0$, $M = 0$). When subjected to a magnetic field, the energy of the singlet state and one of the triplet states is shifted downwards (these two states are called "high-field seekers"), while the energy of the other two states (low-field seekers) is shifted upwards, as shown on Figure 1. During the internship the hyperfine splitting was determined by measuring the transition frequency between the $(F, M) = (1, 0)$ and $(0, 0)$ states (the so-called σ_1 transition) at different external magnetic field values and extrapolating to $B = 0$.

The set-up of the hydrogen beam experiment is sketched in Figure 2. The main components are: the hydrogen source cooled by a cold-head, the permanent sextupole magnet, the chopper, the microwave cavity, the superconducting sextupole magnet, and the quadrupole mass spectrometer (QMS). In the hydrogen source, the hydrogen molecules are broken into atoms which travel through a small aperture forming a thin beam of hydrogen. A decrease in the pressure of the different vacuum chambers of the beamline ensures that hydrogen atoms from the source are pulled towards the strongest vacuum at the QMS at the opposite end. The hydrogen atoms are initially unpolarized with roughly the same number of high- and low-field seekers, but at the permanent sextupole the high-field seekers are deflected, whereas the low-field seekers are focused, resulting in a polarized beam. The chopper periodically blocks the beam off mechanically and so provides a carrier signal that allows the lock-in amplifier to filter out the abundant background hydrogen. As the polarized beam enters the microwave cavity, in which an oscillating magnetic field is produced, the hydrogen atoms

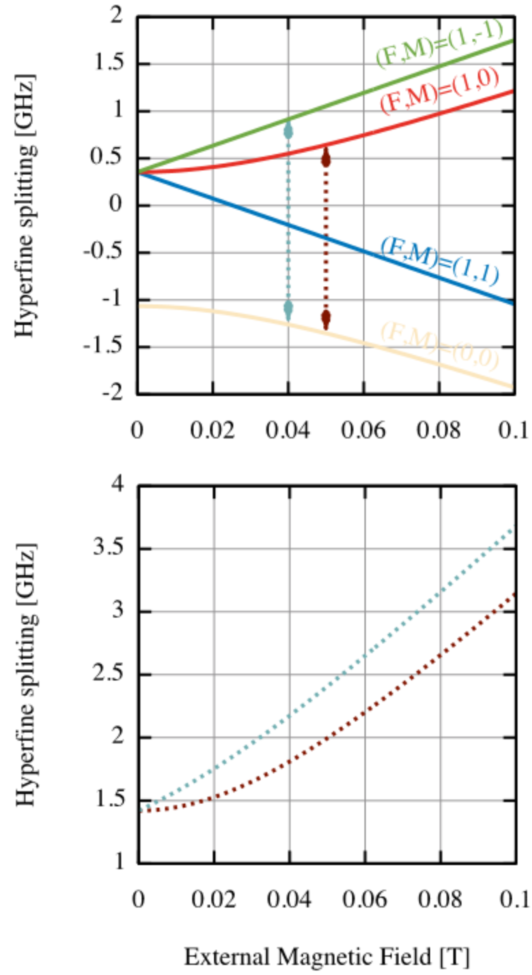


Figure 1: **The hyperfine splitting of the antihydrogen groundstate showing the π_1 transition in cyan and the σ_1 transition in brown. [1]**

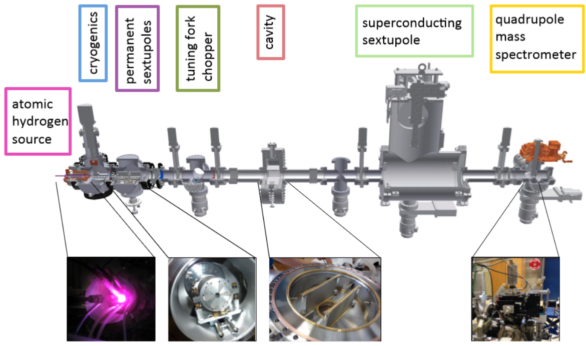


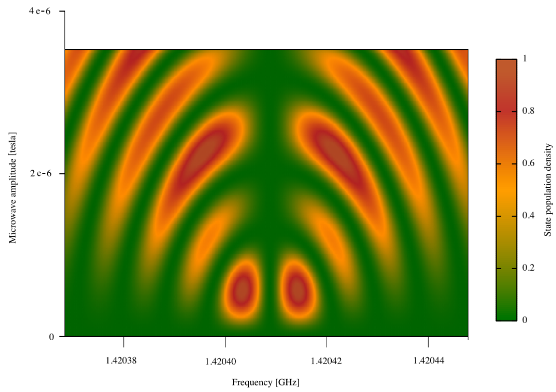
Figure 2: **The experimental set-up of the H-beam experiment. [2]**

undergo Rabi oscillations and a fraction of them have their spins reversed. The cavity is encircled by a pair of Helmholtz coils so that an external homogeneous B-field can be applied inside. On reaching the superconducting sextupole magnet, high-field seekers are once again deflected, and low-field seekers focused, and consequently the converted hydrogen atoms are lost, while the unconverted atoms are detected by the QMS. Since the conversion fraction depends strongly on the transition frequency between the states, the hyperfine splitting of hydrogen can be obtained from the count rate measured by the QMS. The presence of a magnetic field in the microwave cavity despite the magnetic shielding makes a measurement of the hyperfine splitting at zero magnetic field difficult if only one transition (in our case sigma) is measured. That is the reason why the zero-field value is obtained by performing a series of measurements with different constant magnetic fields superimposed onto the oscillating B-field in the cavity and doing a zero-field extrapolation.

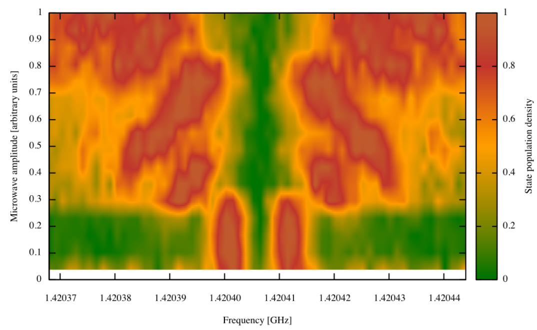
Of the hydrogen beam components, the microwave cavity, which was exchanged with the improved final model in the period from August 5 to 11, and the superconducting sextupole are to be used in the antihydrogen set-up. The characterization of the cavity is therefore of the highest priority for the H-beam experiment and occupied much of the internship.

MICROWAVE CAVITY CHARACTERIZATION

Because of the geometry of the microwave cavity, the expected dependency of the probability that a hydrogen atom is converted on the frequency and amplitude of the B-field in the cavity displays a characteristic two-lobes pattern. Figure 3a shows a simulation of the conversion ratios of hydrogen atoms in a 10 cm long stripline cavity as a function of microwave amplitude and frequency as obtained by numerically solving the optical Bloch equations. To investigate whether the pattern also appears in the experimental data, a 2d scan with the input power varying from 2 to 30 dBm, and the frequency from 1420368000 to 1420444000 Hz, was performed with the new cavity on August 13 to 14 after having optimized the amount of power carried by the oscillating B-field in the cavity. Figure 3b shows the measured count rates after subtracting the value of the lowest count at the respective frequency and then dividing by the value of the largest count so that all values fall between zero and one. It is seen that with the new cavity, the first four conversions are now within reach of the accessible input power.



(a) **Simulation of the state population density of a 10 cm long stripline cavity at 1 Gauss Helmholtz field and 850 m/s. [3]**



(b) **Measured total countrate, subtracted by lowest countrate and then divided by the highest at 50 K.**

FITTING WITH SPLINE-INTERPOLATED SIMULATION

A large part of the work of the internship consisted in developing a routine for fitting the measured lineshape with a weighted sum of cubic splines interpolated from the simulated data as follows:

The simulated data consists of set of conversion ratios distributed on a two-dimensional grid of frequencies f and B-field amplitudes B (fig. 4a). 1d intermediate splines of conversion ratio as a function of amplitude are calculated at every frequency value in the simulated data (fig. 4b); in this way we obtain interpolated data for a continuum of amplitudes and a discrete set of frequencies. We can then perform spline

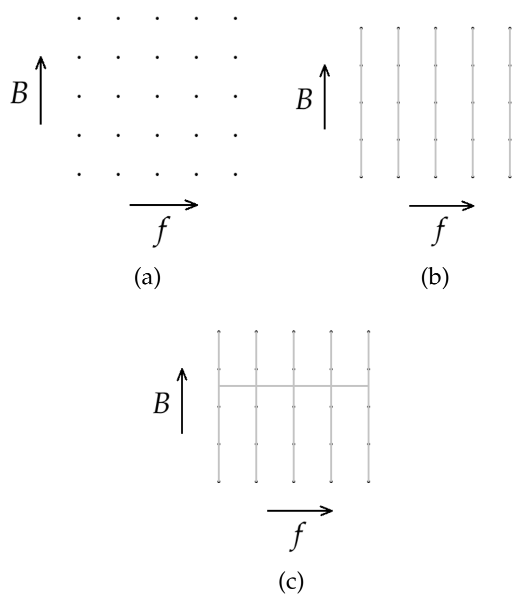


Figure 4: **The steps of the spline interpolation procedure**

interpolation over the discrete set of frequencies to finally obtain a spline of conversion ratios as a function of frequencies for any amplitude (fig. 4c). The simulated data is only valid for a given static magnetic field. However, the amplitude of the static external magnetic field simply shifts the resonance shape along the frequency axis. Therefore, the amplitude of the magnetic field can also be a fitted parameter.

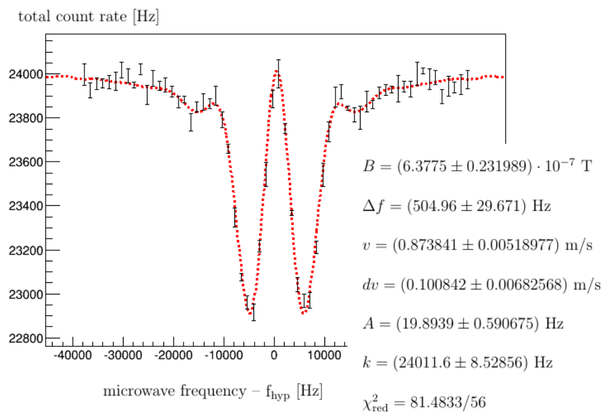
The final spline, then, outputs a population density as a function of frequency f, microwave amplitude B, overall frequency shift Δf, and lastly the velocity v of the hydrogen atoms. The simulated 2d plots depend linearly on v so that data can be obtained for any value of v by merely rescaling the axes by a constant factor. But the simulated data is valid only for hydrogen atoms of a fixed velocity, whereas the hydrogen atoms in the experiment are expected to be distributed roughly according to a Gaussian (not Boltzmann-distributed since the permanent sextupole magnets select a small velocity range within the Boltzmann distribution). In order to take into account this spread in velocities, the lineshape is composed of seven different splines at the same amplitude but interpolated from simulated data valid for different H-atom velocities a distance dv apart, each of which splines is multiplied with a binomial coefficient to approximate the Gaussian distribution:

$$\text{lineshape} = \sum_{n=0}^{6} \binom{6}{n} \text{spline}(f, B, \delta f, v + (n-3)dv)$$

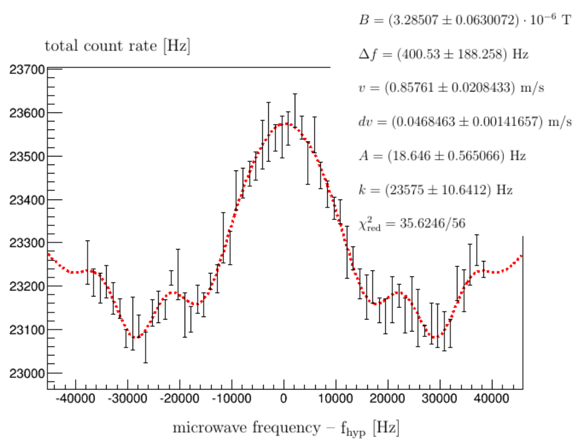
Lastly, the spline sum is multiplied with a factor A to take into account the number of polarized H-atoms present during the measurement, and a constant term k is added to represent the background, so that we arrive at a fit function with six parameters, and with which the beam count of the QMS can be fitted as a function of frequency:

$$\text{fitfun}(f; B, \Delta f, v, dv, A, k) = A \cdot \text{lineshape}(f, B, \Delta f, v, dv) + k$$

So far the fit function so derived has managed to capture the shape of all plots of frequency vs. beam rate on which it has been tested. Two examples are shown on Figures 5a and 5b, where the frequency scans at respective input powers of 14.5 and 30 dBm from Figure 3b have been fitted. By fitting all the frequency scans one finds that the fitted values of B is roughly proportional square root of the input power, as expected, that v is roughly constant, and that dv decreases roughly linearly with the square root of the input power, as is all shown on Figure 6. The range in which the central velocity v fluctuates stretches from 750 to 920 m/s; for comparison, it should be noted that the 2d scan was performed at a coldhead temperature of 50 K, and that the most probable speed for Boltzmann-distributed hydrogen atoms at 50 K is given by $\sqrt{2kT/m} = 911$ m/s. It seen, however, that there is a distinct outlier to these trends, and in fact the second to last values of B, v, and dv were found only after restricting the permitted parameter space so as to exclude an outlier region, where the fit was also converging.



(a) **Frequency scan at 14.5 dBm input power**



(b) **Frequency scan at 30.0 dBm input power**

Figure 5: **Total beam rates fitted as functions of frequency with the new fit routine.**

It is a general problem with the new fit routine that, because of the large variety of different curves it is to encompass, it might converge on local unphysical chi-square minima, which for low-statistics measure-

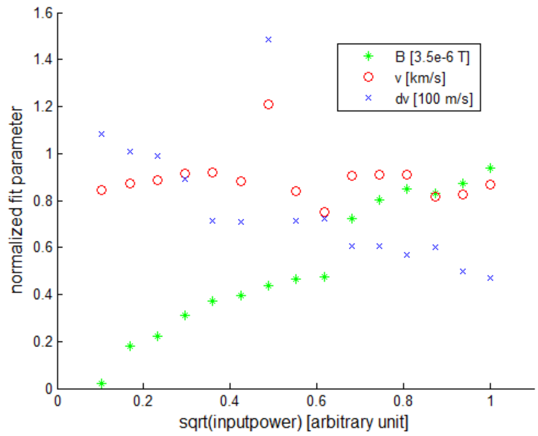


Figure 6: **Fit parameter values from fits of the frequency scans of figure 3b with the new routine.**

ments might even have a lower chi-square than any physical chi-square minimum. Also, if one is not careful to sweep through the parameter space, the fit results obtained exhibit a significant dependency on the initial values of the parameters.

Another issue with the new routine is a rather lengthy computation time in performing a fit (some 15-25 minutes on a personal laptop for a set of 39 datapoints with 5 repetitions each) due to N splines being extrapolated every time the fit function is called.

ZERO-FIELD EXTRAPOLATION OF THE HYPERFINE TRANSITION

Over the summer several sets of frequency scans at different Helmholtz currents were performed in order to test the H-beam setup and obtain the hyperfine splitting transition at zero external magnetic field by extrapolation as explained above. After several optimizations, most importantly aligning the QMS on the beam centre, the best such dataset, consisting of 12 frequency scans similar to the one pictured in Figure 5a, was obtained on August 4. Table I shows the fitted central velocities, their errors, and the chi-squares obtained when fitting the scans with the spline fit routine. From the central frequencies and their errors as a function of the amplitude of the constant B-field generated by the Helmholtz current, the hyperfine transition frequency f_{hyp} has been found by fitting with the following function:

$$f_{\text{cent}} - f_{\text{lit}} = df\sqrt{1+\lambda^2(C\cdot B - B_0)^2} + f_{\text{lit}}\left(\sqrt{1+\lambda^2(C\cdot B - B_0)^2} - 1\right)$$

where C, I_0, and $df \equiv f_{\text{hyp}} - f_{\text{lit}}$, are fit parameters and f_{lit} is the literature value of the transition frequency:[5] $f_{\text{lit}} = 1420405751.7667(10)$ Hz, by which the center frequencies have been shifted in order to work with fewer digits. λ is expressible in terms of the electron and proton g-factors g_e and g_p, the Bohr and proton magneton μ_B and μ_p, the Planck constant h, and the hyperfine transition frequency:

$$\lambda = \left(g_e + g_p\frac{\mu_p}{\mu_B}\right)\frac{\mu_B}{f_{\text{hyp}}h} = 19.7302\ \text{Hz}^{-1} \quad (1)$$

The fit is shown on Figure 7. The fit parameter C reflects the fact that the B-field values used in the fit were measured by flux gates mounted on the outside of the cavity, while the B-field on the inside may have been different. A conversion factor of $B_{\text{in}}/B_{\text{out}} = 0.922(13)$ between the inner B-field value and the readings of the outer flux gate was obtained [4] from previous offline measurements. The value obtained for C from the measurements at different Helmholtz currents is 0.9289 (5) and so agrees with this finding.

As for the hyperfine transition frequency, the zero-point extrapolation fit yields the following value:

$$f_{\text{hyp}} - f_{\text{lit}} = (5.1 \pm 9.1)\ \text{Hz}$$

Table I: **Results from fits of frequency scans**

coil current [mA]	f_{cent} [Hz]	$\sigma_{f_{\text{cent}}}$ [Hz]	χ^2_{red}
-550	1420423431	26	1.51
-450	1420417561	27	1.43
-350	1420412908	31	2.02
-250	1420409438	21	2.69
-150	1420407035	32	1.21
-50	1420405903	25	2.09
50	1420405911	13	1.80
150	1420407031	24	0.74
250	1420409386	31	0.91
350	1420412792	27	0.84
450	1420417480	31	1.39
550	1420423256	27	1.77

With the old lineshape previously used for fitting the frequency scans of the H-beam experiment – a phenomenological analytical expression that was found to reproduce well the simulated data – one arrives at the following value:

$$f_{\text{hyp}} - f_{\text{lit}} = (16.2 \pm 7.9)\ \text{Hz}$$

The reduced chi-squared of the fit with the new fit routing is 1.022, while that of the old lineshape is 1.777.

CONCLUSION

The work of the internship was divided between optimizing the experimental set-up, taking measurements, and developing a new fit routine. One goal was to maximize the power fed through the microwave cavity. The best cavity input port and stub-tuner position was found and enabled the measurement of the first four conversions as shown in Figure 3b. Through lengthy measurements, the shape and

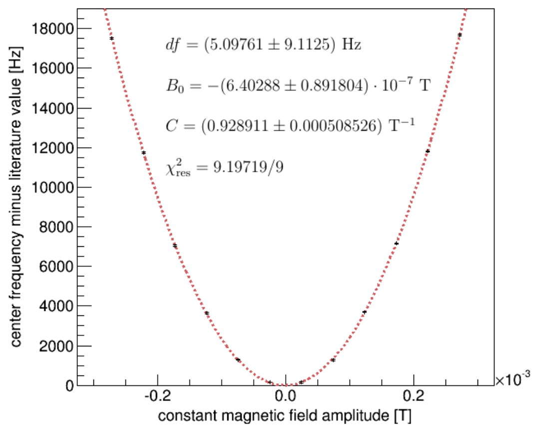


Figure 7: **Fit of resonance center frequency as a function of B-field for zero-field extrapolation.**

locations of the conversions were mapped out at various microwave frequencies and powers, so that diagonal scans through the conversions may be performed with the antihydrogen beam, for which there is insufficient data for a 2d scan.

As for the new fit routine, it has proven capable of fitting the beam rates at all frequencies and powers of interest, and at the cost of an increase in computation time and a greater risk of terminating at local chi-square minima, it yields a more accurate determination of the hyperfine transition frequency of hydrogen than the previous fitting routine and has the added benefit of providing estimates of the power dispersed inside the cavity, of the central velocity of the H-atoms, and of the width of their velocity distribution – physical quantities which are not directly measurable.

As a consequence of the efforts put into achieving the cleanest polarized hydrogen signal possible in conjunction with the application of the new fit function, it was possible to determine the hyperfine transition frequency of hydrogen to within a relative uncertainty of 6 parts per billion.

On a closing note, I should like to express my gratitude to Martin Diermaier and Martin Simon of the Stefan Meyer Institute and to Chloé Malbrunot of CERN, thanks to whose patient guidance this internship became a most rewardful and memorable experience.

[1] Figure by C. Malbrunot, used with permission
[2] Figure by M. Diermaier, used with permission
[3] C. Sauerzopf. Internal communications
[4] C. Heindler. Internal communications
[5] Essen, L et al. (1971) "Frequency of the Hydrogen Maser" Nature, 229 (110).