

Calibration of the Breit-Rabi Polarimeter for the PAX Spin-Filtering Experiment at COSY/Jülich and AD/CERN

by

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ABSTRACT

The PAX (Polarized Antiproton eXperiment) experiment is proposed to polarize a stored antiproton beam for use at the planned High Energy Storage Ring (HESR) of the FAIR facility at GSI (Darmstadt, Germany). The polarization build-up will be achieved by spin-filtering, i.e., by a repetitive passage of the antiproton beam through a polarized atomic hydrogen or deuterium gas target. The experimental setup requires a Polarized Internal gas Target (PIT) surrounded with silicon detectors. The PIT includes an Atomic Beam Source (ABS), the target cell and a Breit-Rabi Polarimeter (BRP).

The first phase of the Spin-Filtering Studies for PAX covers the commissioning of the PIT components and the measurement of an absolute calibration standard for the BRP at the COSY ring in Jülich. The spin-filtering with protons aim at confirming the results of the FILTEX experiment and determine the pp hadronic spin dependent cross sections at 50 MeV. The second phase will be realized in the Antiproton Decelerator ring (AD) at CERN to polarize antiprotons for the first time using spin-filtering.

This diploma thesis summarizes aspects of the polarization and calibration theory based on the hyperfine structure of hydrogen and deuterium, provides the implemented algorithms necessary to solve the calibration and presents the results of the calibration of the BRP. Additionally, the atomic polarization of the hydrogen gas target measured with a prototype openable storage cell is presented and the error analysis is discussed. The effect of the magnetic holding field on the hyperfine state occupancy is examined. Finally, the stability of the polarization between opening cycles of the storage cell and during an ABS nozzle cycle is presented.

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1. INTRODUCTION

1.1. Proton Structure

The proton is the lightest stable baryon (the actual lifetime limit of the proton is $> 10^{33}$ years (Super-Kamiokande Collaboration)[1]). It is composed of three valence quarks (uud)¹. The u and d quarks are members of the lightest of the three families of quarks. The second family contains the strange s and the charm c quark, the third one the bottom b and top t quarks. All six quarks are fermions with spin $\frac{1}{2}$. The positive charge $+1e$ of the proton originates from the fractional quark charges: $q_u = +\frac{2}{3}e$ for the up quark and $q_d = -\frac{1}{3}e$ for the down quark. The quarks are bound by gluons which are massless vector gauge bosons mediating the strong force [2, 3]. The gluons can split into a virtual quark-antiquark pair ($q\bar{q}$), called *sea quarks*[4], which can annihilate back into gluons. The valence quarks and virtual $q\bar{q}$ pairs inside the proton are referred to as charged partons while gluons as electrically neutral partons.

The momentum and spin distribution of the quarks inside the proton are characterized by three fundamental parton distribution functions (PDF)² [5, 6]: the quark momentum density distribution $f(x, Q^2)$, the helicity distribution $\Delta q(x, Q^2)$ and the transversity distribution $h_q(x, Q^2)$. Here the so-called Bjorken x scaling variable $x = \frac{-q^2}{2M\nu}$ is the fraction of the proton momentum carried by the hard-scattering parton; M is the proton mass and $\nu = \frac{q \cdot p}{M} = E - E'$ is the energy loss of the lepton in the proton rest frame; q is the four-momentum of the exchange photon and p is the four-momentum of the proton in its initial state (Fig. 1.1) [7]. In order to work with positive quantities the value $Q^2 = -q^2 = -(k - k')$ is used by convention.

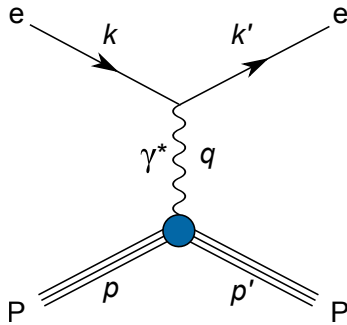


Fig. 1.1.: Feynman diagram for elastic ep collisions [8]. k, k' and p, p' are the four-momenta of the electron and proton before and after the collision respectively. $q = k - k'$ is the four-momentum of the photon (the four-momentum transfer from the electron to the proton).

The nucleon structure has been studied by deep inelastic lepton nucleon scattering (DIS) [7, 9] at SLAC [10, 11], FNAL [12] and CERN [13, 14] and has been measured with great accuracy in the HERA ep collider [15]. Because leptons (electrons, muons, taus) do not feel the strong force they are used as an electromagnetic probe to determine the parton density functions. In an ep collision at a given momentum transfer (or energy scale Q^2 with Q the four-momentum of the exchanged photon) the PDF $f(x, Q^2)$ gives the probability to find a parton of momentum x [16]. The cross section is proportional to the density function $f_i(x, Q^2)$ of a given quark family i with charge e_i :

$$\frac{d\sigma}{dx dQ^2} \propto \sum_i e_i^2 x f_i(x)$$

¹(uud) is the short form for a system of 2 up and 1 down quark.

²The distributions express the probability to find a constituent in a certain state.

The first DIS scattering experiments revealed that not each of the three valence quarks carries one third of the proton momentum³. Instead, almost half of the proton momentum is carried by partons with no electric charge: the gluons [8, 17]. The proton is a fermion with spin $\frac{1}{2}$ and, as a composite particle, the question arises how the spin $\frac{1}{2}$ originates from its constituents. An aim is the decomposition of the longitudinal spin components [18]:

$$\frac{1}{2} = \frac{1}{2} \sum_q \Delta q + \Delta g + L_q + L_g. \quad (1.1)$$

Here Δq and Δg are the longitudinal spin contribution of the quarks and gluons, respectively, and L_q and L_g are the orbital angular momentum contributions. In a longitudinally polarized proton with respect to its momentum, the helicity distribution $\Delta q(x, Q^2)$ describes the probability difference to find a quark with its spin aligned or anti-aligned with respect to the spin of the nucleon [19]. In analogy to $\Delta q(x, Q^2)$, the transversity distribution $h_1^q(x, Q^2)$ describes the difference of the probabilities to find a quark with its spin aligned or anti-aligned to the transversal polarization of the nucleon [20, 21, 22, 23, 24].

The first polarized deep-inelastic muon-proton scattering experiments performed at CERN in the 80s (EMC [25, 26]) have revealed that the valence quarks contribute only 25-30% to the proton spin, instead of 60% predicted by the relativistic quark model. A large part of the spin could be carried by gluons, sea quarks and orbital angular momenta of quarks and gluons [27]. The COMPASS experiment at CERN as well as PHENIX and STAR at RHIC, however, measured a gluon polarization much too small to explain the 30% missing according to the theoretical predictions [28, 29, 30]. Also the sea quark polarization, measured by the HERMES experiment at DESY, indicates that the contribution of the sea quarks to the spin is consistent with zero and can not resolve the spin problem either [31, 32]. All these experiments show that the spin of the valence quark accounts for less than half of the nucleon spin. The missing spin contribution could originate from the orbital angular momenta of the quarks and gluons. In addition to the spin problem the transversity is the last missing PDF necessary to understand the nucleon quark structure [33] and constitutes the main physics motivation for the PAX experiment.

1.2. PAX Experiment

The planned Facility for Antiproton and Ion Research (FAIR) to be build at GSI in Darmstadt [34] will include a High Energy Storage Ring for antiprotons (HESR). The PAX⁴ collaboration proposes a dedicated experiment with polarized antiprotons in an upgrade into a collider [35]. The experiment consists of an Antiproton Polarizer Ring (APR) to polarize antiprotons at energies of 50-250 MeV and a Cooler Synchrotron Ring (CSR) to store protons or antiprotons at energies up to 3.5 GeV. The asymmetric collider consist of a polarized antiproton beam circulating in the HESR (with energies of 1.5-15 GeV) and a polarized proton beam circulating in the CSR, as depicted in Fig. 1.2.

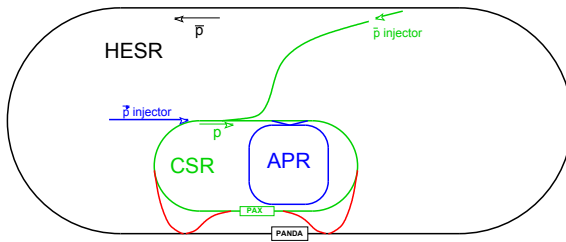


Fig. 1.2.: Proposed HESR accelerator setup for FAIR. The antiprotons are polarized in the APR by spin-filtering. The CSR can store protons or antiprotons up to 3.5 GeV. At the PAX interaction point polarized antiprotons up to 25 GeV from the HESR will collide with polarized protons from the CSR [35] (or vice versa).

³The parton model was introduced to explain these results.

⁴PAX collaboration (Polarized Antiproton EXperiments) see <http://www.fz-juelich.de/ikp/pax>.

A direct way to access the transversity PDF is via the Drell-Yan process with both beams transversely polarized [36, 6]:

$$p^\uparrow + \bar{p}^\uparrow \longrightarrow l^+ + l^- + X$$

where X are the undetected hadrons. The Feynman diagram of the Drell-Yan process is shown in Fig. 1.3.

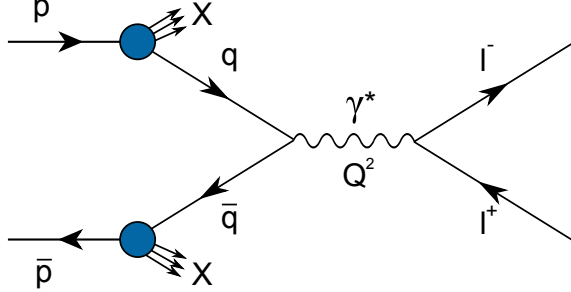


Fig. 1.3.: Drell-Yan process $\bar{p} + p \rightarrow l^+ + l^- + X$. Q is the four-momentum of the photon and Q^2 is also the invariant mass of the lepton pair [6].

The resulting transverse double spin asymmetry A_{TT} involves only the transverse distributions h_1 of the quarks:

$$A_{TT} = \frac{d\sigma^{\uparrow\uparrow} - d\sigma^{\uparrow\downarrow}}{d\sigma^{\uparrow\uparrow} + d\sigma^{\uparrow\downarrow}} = \hat{a}_{TT} \frac{\sum_q e_q^2 h_1^q(x_1, M^2) h_1^{\bar{q}}(x_2, M^2)}{\sum_q e_q^2 h_1^q(x_1, M^2) \bar{q}(x_2, M^2)}$$

with the quark family $q = u, d, \dots$, $\bar{q} = \bar{u}, \bar{d}, \dots$, M the lepton pair invariant mass and $x_{1,2}$ the fractions of the longitudinal momenta of the colliding hadrons which is carried by the annihilating quark and antiquark. The double spin asymmetry $\hat{a}_{TT}$ of the QED process $q\bar{q} \rightarrow l^+l^-$ is given by

$$\hat{a}_{TT} = \frac{\sin^2 \theta}{1 + \cos^2 \theta} \cos 2\phi$$

with θ the polar angle of the l^+l^- lepton pair and ϕ the azimuthal angle between the dilepton direction and the plane defined by the collision and polarization axis [36] in the lepton centre-of-mass frame (see Fig. 1.4).

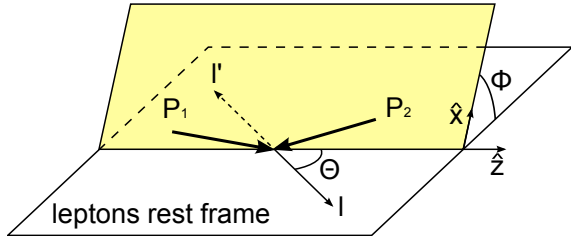


Fig. 1.4.: Drell-Yan process angles in the lepton rest frame. $P_{1,2}$ are the four-momenta of the colliding protons and antiprotons, and l, l' are the four-momenta of the leptons [6].

Polarized $p^\uparrow \bar{p}^\uparrow$ interactions have the potential to measure new fundamental observables which remained inaccessible so far. The crucial prerequisite is to produce a polarized antiproton beam that provides a high luminosity for the experiments. This step will be tested in spin-filtering studies at COSY/Jülich and at AD/CERN.

1.3. Spin-Filtering Studies for PAX

The polarization and storage of an antiproton beam has been tried without success for decades [37]. Out of all methods proposed during the workshop held in Bodega Bay in 1985 [38], the only tested method agreed upon during the recent workshops held in Daresbury in 2007 [39] and Bad Honnef in 2008 [40] is the buildup of polarization by means of spin-filtering [41].

The beam polarization is defined by the relative proportion of antiprotons with spin parallel or anti-parallel to the quantization axis⁵: $P_B = (N_\uparrow - N_\downarrow)/N$; with N the total antiproton population

⁵The quantization axis for the spin orientation is defined by the magnetic holding field.

$N = N_{\uparrow} + N_{\downarrow}$ of the beam and $N_{\uparrow\downarrow}$ the two possible spin states. The principle of spin-filtering is to selectively remove one spin-state of the antiprotons more than the other spin-state from the initially unpolarized beam $N_{\uparrow} = N_{\downarrow}$ using a polarized gas target. Because the total $\bar{p}p$ cross section is different for parallel and anti-parallel orientation of the antiproton spins relative to the direction of the target polarization, the repeated passage of the beam through a polarized gas target results in a beam polarization, increasing with the storage time. This principle can be deduced from the total hadronic cross section [42, 43]:

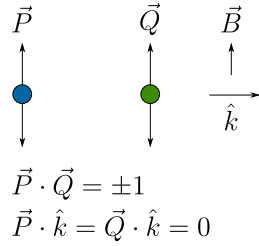
$$\sigma_{tot} = \sigma_0 + \sigma_1(\vec{P} \cdot \vec{Q}) + \sigma_2(\vec{P} \cdot \hat{k})(\vec{Q} \cdot \hat{k}) \quad (1.2)$$

where $\vec{P}$ and $\vec{Q}$ are the vectors of beam and target polarization, σ_0 is the spin-independent hadronic cross section and σ_1, σ_2 are spin-dependent cross sections describing the effect of the relative orientation of $\vec{P}, \vec{Q}$ and the beam direction, given by the unit vector $\hat{k}$. The two cases of transverse and longitudinal polarization are shown in Fig. 1.5. For a fully polarized beam and target, i.e., $|\vec{P}| = 1$ and $|\vec{Q}| = 1$, the cross sections for the transverse and longitudinal cases are⁶

$$\sigma_{tot\pm}^{\perp} = \sigma_0 \pm \sigma_1 \quad \text{and} \quad \sigma_{tot\pm}^{\parallel} = \sigma_0 \pm (\sigma_1 + \sigma_2). \quad (1.3)$$

For an unpolarized beam, the spin orientations $m_{I(P)} = \pm \frac{1}{2}$ are equally populated and the cross sections are calculated with $P = \pm 1$ for $m_{I(P)} = \pm \frac{1}{2}$ and $Q = \pm 1$ for $m_{I(Q)} = \pm \frac{1}{2}$.

transverse polarization



longitudinal polarization

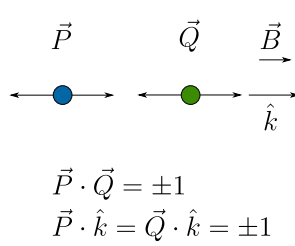


Fig. 1.5.: The relative orientation of proton polarization $\vec{P}$, target polarization $\vec{Q}$, defined by the magnetic holding field $\vec{B}$ and the beam direction (unit vector $\hat{k}$).

Independent switching of the signs of $\vec{P} \cdot \vec{Q}$ and $\vec{Q} \cdot \hat{k}$ between -1 and $+1$ allows to determine σ_1 and σ_2 . The knowledge of their values in the $\bar{p}p$ interaction constitutes the basis to envisage experiments with stored $\bar{p}$ and p beams at FAIR. In addition, the measurement of σ_1 and σ_2 will extend our knowledge about the $\bar{p}p$ system at low energies, which mainly stems from LEAR at CERN [44]. The spin-filtering polarization method has been proven to work for protons in the FILTEX experiment [45] and is now proposed to be reemployed to polarize antiprotons [46].

The spin-filtering Studies for PAX are separated into two phases: the first objective is to test the longitudinal and transverse spin-filtering method and measure the σ_1 and σ_2 observables with protons in the COSY ring in Jülich [47]. The Polarized Internal Target (PIT) and the detection system will be commissioned during this phase. In the second phase, the PIT will be installed in the Antiproton Decelerator ring (AD) at CERN to measure the polarization build-up with antiprotons [48]. This proof of principle will allow the PAX collaboration to define the best parameters for the planned Antiproton Polarizer Ring (APR) at FAIR. Figure 1.6 shows the PIT setup for AD including the quadrupole magnets necessary to form a low- β section. The PIT section consists of an Atomic Beam Source (ABS) to inject a polarized atomic gas, a target chamber hosting a storage cell and a silicon detector system. A so-called Breit-Rabi Polarimeter (BRP) [49] measures the polarization of the target gas.

The σ_1 and σ_2 spin-dependent cross sections are extracted from time constants of the filtering process:

$$\frac{dP}{dt} \propto \frac{1}{\tau_1} \quad \text{with} \quad \tau_1^{\perp} = \frac{1}{\tilde{\sigma}_1 \cdot Q \cdot d_t \cdot f_{rev}} \quad (1.4)$$

⁶(+) for parallel spin and (−) for anti parallel spin.

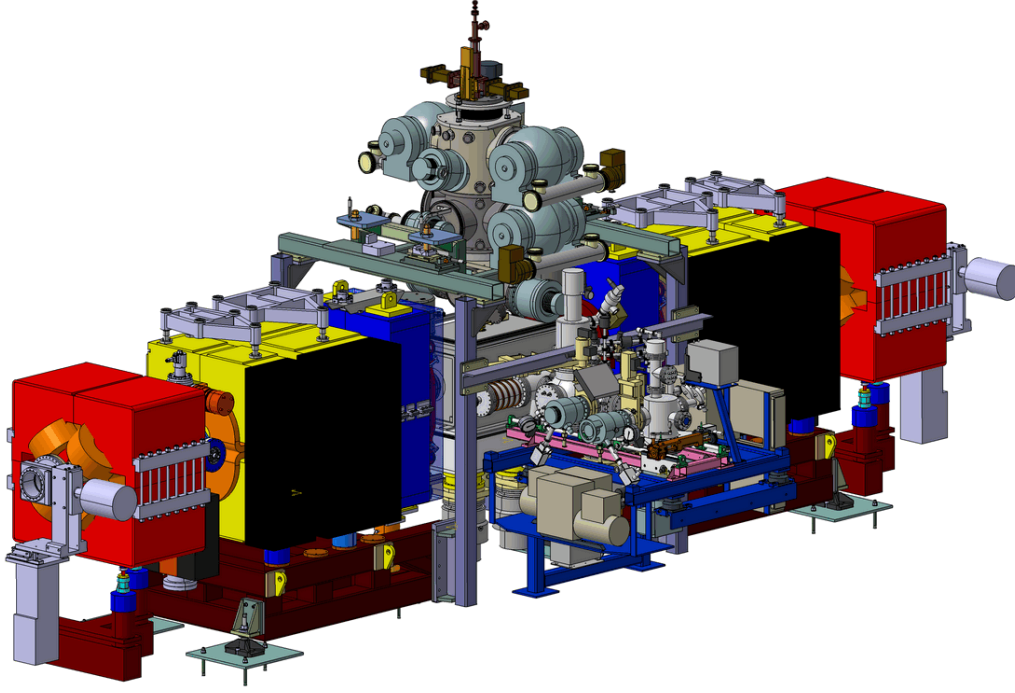


Fig. 1.6.: PAX spin-filtering setup for AD/CERN. The ABS is seen on top, the target chamber hosting the storage cell and the detectors is placed along the beam axis. The BRP is placed off-axis and seen on the right side (source: technical drawing from IKP Forschungszentrum Jülich).

with $\tau_1^\perp$ the transverse time constant, $\tilde{\sigma}_1$ is closely related to σ_1 [46], d_t the target thickness in atoms/cm² and f_{rev} the revolution frequency of the particles. This requires a precise measurement of the beam polarization at the end of a filtering run. As the analyzing power of $p^\uparrow p$ scattering at the experimental energy is negligibly small the beam polarization will be measured by making use of the $p^\uparrow d$ elastic scattering by injecting unpolarized deuterium gas into the storage cell and measuring the left-right scattering asymmetry with the silicon detectors. The reason to use deuterium to measure the polarization of the protons is that the analyzing power is precisely known at the used injection energy (50 MeV) [50] and a clean deuteron selection in the detectors is possible [51].

1.4. Breit-Rabi Polarimeter

The purpose of the Breit-Rabi polarimeter is to measure the target polarization by analyzing a small fraction of the target gas extracted from the storage cell. During the COSY measurements the BRP will monitor the ABS and the storage cell performance. The target gas polarization will be directly measured by $pd^\uparrow$ elastic scattering using the silicon detectors. For the filtering with antiprotons at AD the BRP will provide the calibration standard when the $\bar{p}p$ analyzing power is unknown for the selected energy. Furthermore, with the foreseen spin-filtering using a polarized deuterium target, the BRP will provide the only calibration standard to interpret the measured asymmetries⁷.

The BRP measures the target polarization by determining the relative hyperfine state populations of hydrogen or deuterium atoms [52]. The measurement of the hyperfine state occupancy is based on electron spin-filtering with sextupole magnets and the manipulation of the hyperfine state populations using adiabatic high-frequency transitions. Multiple measurements with different combinations of hyperfine state populations are grouped in a system of equations to extract the hyperfine state populations of the sample.

⁷Filtering with a polarized deuterium target might be more efficient than using hydrogen; however, in this case the $\bar{p}d$ analyzing powers are unknown.

The polarization measurement requires the precise knowledge of the transition efficiencies and the transmission probabilities of the sextupole magnets. These quantities are measured with the BRP calibration. The BRP determines the polarization of the atomic part of the gas sample extracted from the center of the storage cell and the Target Gas Analyzer measures the fraction of atoms and molecules. The polarization, however, is not homogeneous along the storage cell because of differences due to recombination and depolarization on the wall as well as spin-exchange collisions [53, 54]. The actual polarization as seen by the beam is therefore provided only by the detector system which is used to obtain an absolute calibration standard for the BRP.

The objective of this diploma thesis is to develop a procedure to calibrate the BRP. This requires the development of the slow control and data acquisition system and of the offline analysis software and algorithms to extract the calibration values. Chapter 2 provides the theoretical foundation for the hyperfine structure, the hyperfine transitions and the polarization. The working principle of the Breit-Rabi polarimeter and the theory of the polarization measurement, and the algorithms used for the calibration are provided in chapter 3. The experimental setup described in chapter 4 is followed by the calibration measurements and results (chapter 5). Finally, the polarization measurements are presented in chapter 6. Additional operational parameters and the description of the developed software are provided in the appendices.

2. THEORETICAL FOUNDATIONS

2.1. Hyperfine Structure

The Proton, like the electron, is a fermion with spin[&] quantum number $s = 1/2$. The hyperfine structure is the result of the interaction between the magnetic moments of the electron and the nucleus [55, 56, 57, 58, 59, 60, 61, 62]. The nuclear polarization of hydrogen and deuterium as well as the working principles of the ABS and the BRP are based on the hyperfine structure. The nuclear spin observable $\mathbf{I}$ has an associated intrinsic dipole moment of

$$\boldsymbol{\mu}_I = \frac{g_p \mu_N}{\hbar} \mathbf{I} \quad \text{with} \quad \mu_N = \frac{e \hbar}{2 m_p}, \quad (2.1)$$

with the proton gyromagnetic ratio $g_p \simeq 5,585^*$ and m_p the proton mass. The magnetic moment of the proton generates a magnetic field [63]:

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi r^3} \left[3(\boldsymbol{\mu}_p \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}} - \boldsymbol{\mu}_p \right] + \frac{2\mu_0}{3} \boldsymbol{\mu}_p \delta^3(\mathbf{r}) \quad (2.2)$$

with $\hat{\mathbf{r}} = \mathbf{r}/r$. The first term in (2.2) originates from the classical magnetic dipole. The second term can be explained by visualizing the proton magnetic dipole as a tiny current loop. All magnetic field lines generated by the loop must be closed. However, the magnetic field approaches infinity when the loop size goes to zero. This effect is reflected by the delta function.[56, 64]

The electron immersed in the magnetic field produced by the proton has the following Hamiltonian:

$$\mathcal{H}_{HFS} = -\boldsymbol{\mu}_S \cdot \mathbf{B}. \quad (2.3)$$

The electron intrinsic magnetic moment generated by its spin is:

$$\boldsymbol{\mu}_S = -\frac{g_s e}{2 m_e} \mathbf{S}, \quad (2.4)$$

with the electron gyromagnetic ratio $g_s \approx 2.002^*$ and the electron spin $\mathbf{S} = \pm \frac{\hbar}{2}$. In the electron ground state with $l = 0$ the coupling of the proton spin with the electron orbital angular momentum can be neglected. With equations (2.1), (2.2) and (2.3) the Hamiltonian perturbing the ground state is given by:

$$\mathcal{H}_{HFS} = \frac{\mu_0 g_s g_p e^2}{16\pi m_p m_e} \frac{3(\mathbf{I} \cdot \hat{\mathbf{r}})(\mathbf{S} \cdot \hat{\mathbf{r}}) - \mathbf{I} \cdot \mathbf{S}}{r^3} + \frac{\mu_0 g_s g_p e^2}{6 m_p m_e} \mathbf{I} \cdot \mathbf{S} \delta^3(\mathbf{r}). \quad (2.5)$$

The magnetic moment of the proton being smaller than that of the electron by a factor of the order m_e/m_p , the effect of the hyperfine structure can be treated as a perturbation. The first order of the perturbation theory is the expectation value of the perturbing Hamiltonian:

$$\Delta E = \frac{\mu_0 g_s g_p e^2}{16\pi m_p m_e} \left\langle \frac{3(\mathbf{I} \cdot \hat{\mathbf{r}})(\mathbf{S} \cdot \hat{\mathbf{r}}) - \mathbf{I} \cdot \mathbf{S}}{r^3} \right\rangle + \frac{\mu_0 g_s g_p e^2}{6 m_p m_e} \langle \mathbf{I} \cdot \mathbf{S} \rangle |\psi|^2. \quad (2.6)$$

[&]The spin is in units of $\hbar$ (the reduced Planck constant $\hbar = h/2\pi$).

* see appendix H for precise numerical values.

Because the wavefunction ψ is spherically symmetric in the ground state, the first term in (2.6) vanishes and only the term with the delta function in (2.5) contributes in the spin-spin Hamiltonian. With the first normalized wavefunction for the hydrogen ground state [65, 66]:

$$\psi_{100} = \frac{e^{-r/a_0}}{\sqrt{\pi} a_0^{3/2}}; \quad \text{and} \quad |\psi_{100}|^2 = \frac{1}{\pi a_0^3}, \quad (2.7)$$

and with the Bohr radius

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \frac{\hbar}{m_e c \alpha}, \quad (2.8)$$

the energy difference becomes

$$\Delta E_{HFS} = \mathcal{A}_H \langle \mathbf{I} \cdot \mathbf{S} \rangle \quad \text{with} \quad \mathcal{A}_H = \frac{\mu_0 g_s g_p e^2}{6\pi m_p m_e a_0^3}. \quad (2.9)$$

Using (2.8) and $\mu_0 = 1/\epsilon_0 c^2$ the so-called contact term $\mathcal{A}_H$ describing the spin-spin coupling strength can be written as

$$\mathcal{A}_H = \frac{2}{3} \frac{e^2 g_s g_p}{\hbar^2} \frac{m_e^2}{m_p} c^2 \alpha^4, \quad (2.10)$$

where α is the fine-structure constant $\alpha = e^2/4\pi\epsilon_0\hbar c \approx 1/137$. The product $\langle \mathbf{I} \cdot \mathbf{S} \rangle$ can be calculated using the total angular momentum $\mathbf{F}$ (with $\mathbf{L} = 0$):

$$\mathbf{F} = \mathbf{S} + \mathbf{I}, \quad (2.11)$$

leading to

$$F^2 = S^2 + I^2 + 2(\mathbf{I} \cdot \mathbf{S}) \Rightarrow \mathbf{I} \cdot \mathbf{S} = \frac{1}{2}(F^2 - S^2 - I^2). \quad (2.12)$$

The total angular momentum operators F^2 and F_z with the new quantum numbers F and m_F commute with the Hamiltonian (2.5) since the operator $\langle \mathbf{I} \cdot \mathbf{S} \rangle$ is represented by the basis $\{|F, m_F\rangle\}$. Therefore, the states $|F, m_F\rangle$ are eigenstates of $\mathcal{A}_H \mathbf{I} \cdot \mathbf{S}$. With the classical angular momentum relations

$$F^2|\psi\rangle = F(F+1)\hbar^2|\psi\rangle \quad (2.13)$$

$$F_z|\psi\rangle = m_F\hbar|\psi\rangle, \quad (2.14)$$

and with (2.12) this leads to

$$\begin{aligned} \mathcal{A}_H \mathbf{I} \cdot \mathbf{S} |F, m_F\rangle &= \frac{\mathcal{A}_H \hbar^2}{2} [F(F+1) - I(I+1) - S(S+1)] |F, m_F\rangle \\ &= \frac{\mathcal{A}_H \hbar^2}{2} [F(F+1) - \frac{3}{2}] |F, m_F\rangle. \end{aligned} \quad (2.15)$$

The eigenstates of (2.15) only depend on the quantum number F and not on m_F . The net state of the addition of two spin 1/2 particles has either spin 1 or spin 0 with possible values for $F = 0, 1$. The three states with spin 1 and possible values for $m_F = -1, 0, 1$ are known as triplet states, and the spin 0 state is the singlet state. The energies eigenvalues are

$$\mathcal{A}_H \mathbf{I} \cdot \mathbf{S} = \frac{\mathcal{A}_H}{4} \hbar^2 \quad \text{for} \quad F = 1 \quad (2.16)$$

$$\mathcal{A}_H \mathbf{I} \cdot \mathbf{S} = -\frac{3\mathcal{A}_H}{4} \hbar^2 \quad \text{for} \quad F = 0. \quad (2.17)$$

Therefore, the fourfold degeneration of the ground state $1S_{1/2}$ is broken and the energies are split into two levels; the level $F = 1$ is threefold degenerated. This splitting is known as the hyperfine

structure and is calculated with (2.9) and (2.8). It induces a net energy difference between the triplet and singlet states of:

$$\Delta E_{HFS} = \frac{8}{3} g_p \frac{m_e}{m_p} \alpha^2 E_0 \simeq 5.88 \times 10^{-6} \text{ eV}, \quad (2.18)$$

with the ground state energy $E_0 = 13.6 \text{ eV}$ for hydrogen. The corresponding frequency is*

$$\nu_{HFS} = \frac{\mathcal{A}_H \hbar}{2\pi} \simeq 1420 \text{ MHz} \quad (2.19)$$

and the radiation wavelength

$$\lambda_{HFS} = \frac{c}{\nu} \simeq 21.1 \text{ cm}. \quad (2.20)$$

Without external magnetic field or in a weak magnetic field with $B \ll B_C$ the basis $\{|F, m_F\rangle\}$ is used to describe the four hyperfine states:

$$\begin{aligned} |i\rangle &= |F, m_F\rangle \rightarrow |m_S, m_I\rangle \\ |1\rangle &= |1, +1\rangle = \left|+\frac{1}{2}, +\frac{1}{2}\right\rangle \\ |2\rangle &= |1, 0\rangle = \frac{1}{\sqrt{2}} \cdot \left(\left|+\frac{1}{2}, -\frac{1}{2}\right\rangle + \left|-\frac{1}{2}, +\frac{1}{2}\right\rangle\right) \\ |3\rangle &= |1, -1\rangle = \left|-\frac{1}{2}, -\frac{1}{2}\right\rangle \\ |4\rangle &= |0, 0\rangle = \frac{1}{\sqrt{2}} \cdot \left(\left|+\frac{1}{2}, -\frac{1}{2}\right\rangle - \left|-\frac{1}{2}, +\frac{1}{2}\right\rangle\right). \end{aligned} \quad (2.21)$$

The states $|2\rangle$ and $|4\rangle$ are a mixing of the eigenstates with the quantum numbers m_S and m_I from the basis $\{|m_S, m_I\rangle\}$ see Eq. (2.34) below.

For deuterium, the nucleus having a spin 1, the quantum numbers for the total angular momenta are $F = \frac{3}{2}, \frac{1}{2}$, also corresponding to two energy levels in the ground state. The state $F = \frac{3}{2}$ is a quadruplet with $m_F = -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}$, and the state $F = \frac{1}{2}$ is a doublet with $m_F = -\frac{1}{2}, +\frac{1}{2}$. The spin-spin coupling strength is given by:

$$\mathcal{A}_D = \frac{2}{3} \frac{e^2 g_s g_d}{\hbar^2} \frac{m_e^2}{m_p} c^2 \alpha^4, \quad (2.22)$$

with the deuteron g-factor $g_d \simeq 0.857^*$. The hyperfine energy splitting has the value of

$$\Delta E_{HFS} = \frac{3}{2} \mathcal{A}_D \hbar^2 \simeq 1.35 \times 10^{-6} \text{ eV} \quad (2.23)$$

with the corresponding frequency

$$\nu_{HFS} = \frac{\mathcal{A}_D \hbar}{2\pi} \simeq 327.4 \text{ MHz}. \quad (2.24)$$

2.2. Zeeman Splitting

When the atom is immersed in a static magnetic field B_z in the z direction, the field will interact with the magnetic moments of the electron spin as well as the angular momentum of the electron and the nucleon spin [55, 67, 68]:

$$\boldsymbol{\mu}_S = -\frac{e g_s}{2m_e} \mathbf{S}, \quad \boldsymbol{\mu}_L = -\frac{e}{2m_e} \mathbf{S} \quad \text{and} \quad \boldsymbol{\mu}_I = \frac{e g_p}{2m_p} \mathbf{I}. \quad (2.25)$$

The Zeeman Hamiltonian is given by the interaction between the magnetic moments (2.25) and the external field:

$$\mathcal{H}_z = -\mathbf{B}_z \cdot (\boldsymbol{\mu}_S + \boldsymbol{\mu}_L + \boldsymbol{\mu}_I) \quad (2.26)$$

The angular momentum term can be ignored for the ground state ($l = 0$). Using the Bohr and nuclear magneton relations

$$\mu_B = -\frac{e\hbar}{2m_e} \quad \text{and} \quad \mu_N = -\frac{e\hbar}{2m_p}, \quad (2.27)$$

the hyperfine Hamiltonian in a magnetic field, together with the spin-spin term (2.9) is given by [69]

$$\mathcal{H}_{HFSz} = \mathcal{A}_{H,D} \mathbf{S} \cdot \mathbf{I} + \frac{g_S \mu_B}{\hbar} \mathbf{S} \cdot \mathbf{B} - \frac{g_I \mu_N}{\hbar} \mathbf{I} \cdot \mathbf{B} \quad (2.28)$$

Using $\epsilon_H = \frac{g_I \mu_N}{g_S \mu_B} = 1.5 \times 10^{-3} \ll 1$ for hydrogen and $\epsilon_D = \frac{g_I \mu_D}{g_S \mu_B} = 2.3 \times 10^{-4} \ll 1$ for deuterium the static¹ Hamiltonian (2.28) can be written as [70, 71, 55, 72]

$$\mathcal{H}_H^{st} = \mathcal{A}_H \hbar^2 \left[\frac{\mathbf{S} \cdot \mathbf{I}}{\hbar^2} + \frac{\mathbf{B}}{B_C^H} \cdot \left(\frac{\mathbf{S}}{\hbar} - \epsilon_H \frac{\mathbf{I}}{\hbar} \right) \right] \quad \text{for hydrogen} \quad (2.29)$$

and

$$\mathcal{H}_D^{st} = \mathcal{A}_D \hbar^2 \left[\frac{\mathbf{S} \cdot \mathbf{I}}{\hbar^2} + \frac{3}{2} \frac{\mathbf{B}}{B_C^D} \cdot \left(\frac{\mathbf{S}}{\hbar} - \epsilon_D \frac{\mathbf{I}}{\hbar} \right) \right] \quad \text{for deuterium.} \quad (2.30)$$

$B_C^H = \frac{\mathcal{A}_H \hbar}{g_S \mu_B} \simeq 50.7$ mT and $B_C^D = \frac{2}{3} \frac{\mathcal{A}_D \hbar}{g_S \mu_B} \simeq 11.7$ mT are the so-called *critical fields* of hydrogen and deuterium, respectively.

The spin-spin coupling term $\mathbf{S} \cdot \mathbf{I}$ and the terms responsible for the interaction with the external field $\mathbf{S} \cdot \mathbf{B}$ and $\mathbf{I} \cdot \mathbf{B}$ in (2.29) can be written as

$$\mathbf{S} \cdot \mathbf{I} = I_z S_z + \frac{1}{2} (I_+ S_- + I_- S_+) \quad (2.31)$$

$$\mathbf{S} \cdot \mathbf{B} = S_z B_z + \frac{1}{2} S_+ (B_x - i B_y) + \frac{1}{2} S_- (B_x + i B_y) \quad (2.32)$$

$$\mathbf{I} \cdot \mathbf{B} = I_z B_z + \frac{1}{2} I_+ (B_x - i B_y) + \frac{1}{2} I_- (B_x + i B_y) \quad (2.33)$$

with $I_{\pm} = I_x \pm i I_y$ and $S_{\pm} = S_x \pm i S_y$.

The states $|m_S, m_I\rangle^2$ form the basis $\{|m_S, m_I\rangle\}$

$$|+\frac{1}{2}, +\frac{1}{2}\rangle, |+\frac{1}{2}, -\frac{1}{2}\rangle, |-\frac{1}{2}, -\frac{1}{2}\rangle, |-\frac{1}{2}, +\frac{1}{2}\rangle \quad \text{for hydrogen} \quad (2.34)$$

and

$$|+\frac{1}{2}, 1\rangle, |+\frac{1}{2}, 0\rangle, |+\frac{1}{2}, -1\rangle, |-\frac{1}{2}, 1\rangle, |-\frac{1}{2}, 0\rangle, |-\frac{1}{2}, -1\rangle \quad \text{for deuterium.} \quad (2.35)$$

Using the above basis and with $S_z = I_z = \pm \frac{\hbar}{2}$, the dimensionless magnetic scaling value $x = B/B_C^{H,D}$, and limiting the magnetic field direction to the z-axis $\mathbf{B} = (0, 0, B)$, the terms in (2.31) are better represented in matrix notation with

$$\mathbf{S} \cdot \mathbf{I} = \frac{\hbar}{4} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 2 \\ 0 & 0 & 1 & 0 \\ 0 & 2 & 0 & -1 \end{pmatrix}, \quad \frac{\mathbf{B}}{B_C^H} \cdot \mathbf{S} = \frac{\hbar}{2} \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & -x & 0 \\ 0 & 0 & 0 & -x \end{pmatrix}, \quad \frac{\mathbf{B}}{B_C^H} \cdot \mathbf{I} = \frac{\hbar}{2} \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & -x & 0 & 0 \\ 0 & 0 & -x & 0 \\ 0 & 0 & 0 & x \end{pmatrix}. \quad (2.36)$$

For deuterium, the matrices are

$$\mathbf{S} \cdot \mathbf{I} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & -1 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad (2.37)$$

¹Static Hamiltonian because all variables are time independent.

²the quantum numbers m_S, m_I refer to the angular momentum operators S_z and I_z .

$$\frac{3}{2} \frac{\mathbf{B}}{B_C^D} \cdot \mathbf{S} = \frac{3}{2} \frac{\hbar}{2} \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & 0 \\ 0 & 0 & 0 & -x & 0 & 0 \\ 0 & 0 & 0 & 0 & -x & 0 \\ 0 & 0 & 0 & 0 & 0 & -x \end{pmatrix}, \quad \frac{3}{2} \frac{\mathbf{B}}{B_C^D} \cdot \mathbf{I} = \frac{3}{2} \hbar \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -x & 0 & 0 & 0 \\ 0 & 0 & 0 & -x & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -x \end{pmatrix}. \quad (2.38)$$

The static Hamiltonian $\mathcal{H}_H^{st}$ (and $\mathcal{H}_D^{st}$) of the hyperfine structure in a magnetic field can now be written in matrix form:

$$\mathcal{H}_H^{st} = \begin{pmatrix} 1 + 2x(1 - \epsilon_H) & 0 & 0 & 0 \\ 0 & -1 + 2x(1 + \epsilon_H) & 0 & 2 \\ 0 & 0 & 1 - 2x(1 - \epsilon_H) & 0 \\ 0 & 2 & 0 & -1 - 2x(1 + \epsilon_H) \end{pmatrix} \quad (2.39)$$

and

$$\mathcal{H}_D^{st} = \begin{pmatrix} 1 + \frac{3}{2}x(1 - 2\epsilon_D) & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2}x & 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & -1 + \frac{3}{2}x(1 + 2\epsilon_D) & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 1 - \frac{3}{2}x(1 - 2\epsilon_D) & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & -\frac{3}{2}x & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & -1 - \frac{3}{2}x(1 + 2\epsilon_D) \end{pmatrix} \quad (2.40)$$

Because the matrices (2.39) and (2.40) are not diagonal, the basis (2.34) and (2.35) are not eigenstates of the Hamiltonians (2.29) and (2.30). Eigenstates and eigenvalues of (2.29) and (2.30) are found by diagonalizing the Hamiltonian with an orthogonal transformation:

$$\mathcal{H}_{diag}^{st} = \mathbf{U}_0^T \mathcal{H}_{H,D}^{st} \mathbf{U}_0. \quad (2.41)$$

The transformation matrices $\mathbf{U}_0^{H,D}$ for hydrogen and deuterium are given by

$$\mathbf{U}_0^H = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & 0 & -\sin \theta \\ 0 & 0 & 1 & 0 \\ 0 & \sin \theta & 0 & \cos \theta \end{pmatrix} \quad \text{and} \quad \mathbf{U}_0^D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos \theta_+ & 0 & 0 & 0 & -\sin \theta_+ \\ 0 & 0 & \cos \theta_- & 0 & -\sin \theta_- & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sin \theta_- & 0 & \cos \theta_- & 0 \\ 0 & \sin \theta_+ & 0 & 0 & 0 & \cos \theta_+ \end{pmatrix}. \quad (2.42)$$

The so-called *mixing angle* θ depends on the magnetic field $x = B/B_C$. The mixing coefficients of $\mathbf{U}_0^{H,D}$ are given in Table 2.1. In the bases (2.34) and (2.35) the eigenvectors of $\mathcal{H}_{H,D}^{st}$ are given in Table 2.2.

The energies of the hyperfine structure in a magnetic field are the eigenvalues of the Hamiltonian $\mathcal{H}_{H,D}^{st}$. The eigenvalues are calculated with (2.41) and are given in Table 2.3. The dependence of the hyperfine energies in respect to the external magnetic field is plotted in Fig. 2.1. This energy splitting is crucial for the target (gas) polarization definition and for the operation of the Breit-Rabi polarimeter. The coupling of the electron and proton spin and thus the polarization of the mixed states is affected by the external magnetic field.

2.3. Polarization of Hydrogen and Deuterium

The proton (electron) polarization P_z (P_e) is defined by the probability to measure the spin parallel or anti-parallel to the magnetic holding field. The expectation value for the nuclear (electron)

Table 2.1.: Mixing coefficients of the hyperfine splitting in a magnetic field for hydrogen and deuterium.

Hydrogen	Deuterium
$\cos \theta = \sqrt{\frac{1}{2}(1 + \cos 2\theta)}$	$\cos \theta_{\pm} = \sqrt{\frac{1}{2}(1 + \cos 2\theta_{\pm})}$
$\sin \theta = \sqrt{\frac{1}{2}(1 - \cos 2\theta)}$	$\sin \theta_{\pm} = \sqrt{\frac{1}{2}(1 - \cos 2\theta_{\pm})}$
$\cos 2\theta = \frac{x(1 + \epsilon_H)}{\sqrt{x^2(1 + \epsilon_H)^2 + 1}}$	$\cos 2\theta_{\pm} = \frac{3x(1 + 2\epsilon_D) \pm 1}{\sqrt{(3x(1 + 2\epsilon_D) \pm 1)^2 + 8}}$
$\sin 2\theta = \frac{1}{\sqrt{x^2(1 + \epsilon_H)^2 + 1}}$	$\sin 2\theta_{\pm} = \frac{\sqrt{8}}{\sqrt{(3x(1 + 2\epsilon_D) \pm 1)^2 + 8}}$

Table 2.2.: The eigenvectors of $\mathcal{H}_{H,D}^{st}$ in the basis $\{|m_S, m_I\rangle\}$ form the so-called Breit-Rabi basis valid for all magnetic fields.

Hydrogen	Deuterium
$ 1\rangle = +\frac{1}{2}, +\frac{1}{2}\rangle$	$ 1\rangle = +\frac{1}{2}, +1\rangle$
$ 2\rangle = \cos \theta +\frac{1}{2}, -\frac{1}{2}\rangle + \sin \theta -\frac{1}{2}, +\frac{1}{2}\rangle$	$ 2\rangle = \cos \theta_+ +\frac{1}{2}, 0\rangle + \sin \theta_+ -\frac{1}{2}, +1\rangle$
$ 3\rangle = -\frac{1}{2}, -\frac{1}{2}\rangle$	$ 3\rangle = \cos \theta_- +\frac{1}{2}, -1\rangle + \sin \theta_- -\frac{1}{2}, 0\rangle$
$ 4\rangle = -\sin \theta +\frac{1}{2}, -\frac{1}{2}\rangle + \cos \theta -\frac{1}{2}, +\frac{1}{2}\rangle$	$ 4\rangle = -\frac{1}{2}, -1\rangle$
	$ 5\rangle = -\sin \theta_- +\frac{1}{2}, -1\rangle + \cos \theta_- -\frac{1}{2}, 0\rangle$
	$ 6\rangle = -\sin \theta_+ +\frac{1}{2}, 0\rangle + \cos \theta_+ -\frac{1}{2}, +1\rangle$

Table 2.3.: Energies eigenstates of the hyperfine splitting in a magnetic field for hydrogen and deuterium.

Hydrogen	Deuterium
$E_1 = \frac{\mathcal{A}_H \hbar^2}{4} (1 + 2x(1 - \epsilon))$	$E_1 = \frac{\mathcal{A}_D \hbar^2}{3} (1 + \frac{3}{2}x(1 - 2\epsilon))$
$E_2 = \frac{\mathcal{A}_H \hbar^2}{4} (-1 + 2\sqrt{x^2(1 + \epsilon)^2 + 1})$	$E_2 = \frac{\mathcal{A}_D \hbar^2}{6} (-1 + \sqrt{9x^2(1 + 2\epsilon)^2 + 6x(1 + 2\epsilon) + 9})$
$E_3 = \frac{\mathcal{A}_H \hbar^2}{4} (1 - 2x(1 - \epsilon))$	$E_3 = \frac{\mathcal{A}_D \hbar^2}{6} (-1 + \sqrt{9x^2(1 + 2\epsilon)^2 - 6x(1 + 2\epsilon) + 9})$
$E_4 = \frac{\mathcal{A}_H \hbar^2}{4} (-1 - 2\sqrt{x^2(1 + \epsilon)^2 + 1})$	$E_4 = \frac{\mathcal{A}_D \hbar^2}{3} (1 - \frac{3}{2}x(1 - 2\epsilon))$
	$E_5 = \frac{\mathcal{A}_D \hbar^2}{6} (-1 - \sqrt{9x^2(1 + 2\epsilon)^2 - 6x(1 + 2\epsilon) + 9})$
	$E_6 = \frac{\mathcal{A}_D \hbar^2}{6} (-1 + \sqrt{9x^2(1 + 2\epsilon)^2 + 6x(1 + 2\epsilon) + 9})$

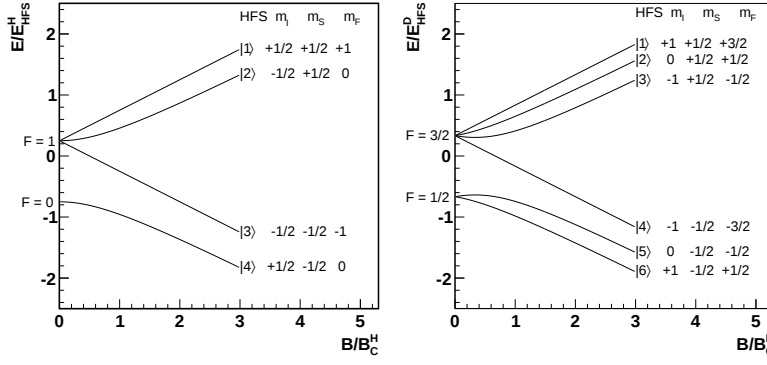


Fig. 2.1.: Breit-Rabi diagram for hydrogen and deuterium normalized to the critical field $x = B/B_C^{H,D}$. Energies eigenstates are given in Table 2.3.

polarization depends on the individual hyperfine state population of the hydrogen or deuterium atoms.

The polarization of a sample of atoms is calculated with the density matrix[73, 74, 75]

$$\rho = \sum_i p_i |\psi^{(i)}\rangle \langle \psi^{(i)}| \quad (2.43)$$

where p_i is the probability to measure the state $|\psi^{(i)}\rangle$ in the sample. The expectation value of an operator $\mathcal{A}$ is given by

$$\langle \mathcal{A} \rangle = \sum_i p_i \langle \psi^{(i)} | \mathcal{A} | \psi^{(i)} \rangle = \text{Tr}(\rho \mathcal{A}). \quad (2.44)$$

The expectation values for the polarization for each individual hyperfine state is given by the basis of eigenvectors in Table 2.2. With this basis $\{|i\rangle\}$ the polarization of the hydrogen or deuterium atomic gas sample is given by

$$P_{e,z} = \sum_i^{4,6} n_i \langle i | \mathcal{P}_{e,z} | i \rangle \quad (2.45)$$

whereby the operator $\mathcal{P}_{e,z}$ is either the operator $\frac{\hbar}{2} S_z$ for the electron or $\frac{\hbar}{2} I_z$ for the proton polarization.

2.3.1. Hydrogen Polarization

Spin $\frac{1}{2}$ particles are described with the Pauli matrices [73, 76]:

$$\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma} \text{ with } \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.46)$$

The eigenstates of S_z are given by the spinor $|\chi\rangle = c_1|+\rangle + c_2|-\rangle$ where c_1 (c_2) is the probability to measure the spin in the positive (negative) direction. It follows that $c_1^2 + c_2^2 = 1$. Using the basis of 2.2 with (2.45) and (2.46) the expectation values for P_z are explicitly given by³:

$$P_{z|1} = \langle 1 | \frac{\hbar}{2} I_z | 1 \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 \quad (2.47)$$

$$P_{z|2} = \langle 2 | \frac{\hbar}{2} I_z | 2 \rangle = \begin{pmatrix} \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sin \theta \\ \cos \theta \end{pmatrix} = -\cos 2\theta \quad (2.48)$$

$$P_{z|3} = \langle 3 | \frac{\hbar}{2} I_z | 3 \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -1 \quad (2.49)$$

$$P_{z|4} = \langle 4 | \frac{\hbar}{2} I_z | 4 \rangle = \begin{pmatrix} \cos \theta & -\sin \theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos \theta \\ -\sin \theta \end{pmatrix} = \cos 2\theta. \quad (2.50)$$

³Using the trigonometric relations $\cos^2 \theta + \sin^2 \theta = 1$ and $\cos 2\theta = \cos^2 \theta - \sin^2 \theta$.

Using (2.45) and (2.47) to (2.50), the expectation value of the polarization which depends on the hyperfine state relative occupation number n_i is defined by:

$$P_z = \sum_{i=1}^4 \langle i | \frac{2}{\hbar} I_z | i \rangle = n_1 - n_3 - (n_2 - n_4) \cos 2\theta \quad (2.51)$$

$$P_e = \sum_{i=1}^4 \langle i | \frac{2}{\hbar} S_z | i \rangle = n_1 - n_3 + (n_2 - n_4) \cos 2\theta \quad (2.52)$$

The relative occupation numbers follow the normalization

$$\sum_{i=1}^4 n_i = 1. \quad (2.53)$$

Using the mixing coefficients of Table 2.1 (Fig. C.1), the polarization of the hydrogen hyperfine states can be calculated as function of B/B_C^H (Fig. 2.2).

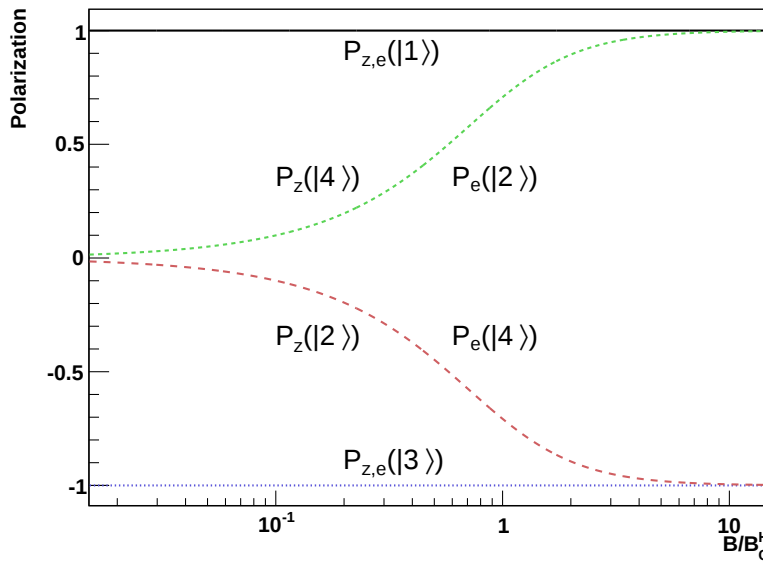


Fig. 2.2.: Polarization of the hyperfine states of hydrogen versus the external magnetic field normalized to the critical field.

For strong fields $B \gg B_C^H$, in the so-called Paschen-Back region the coupling of the electron and proton spin is weak. The sample polarization can be simplified as:

$$P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} = n_{\uparrow} - n_{\downarrow}, \quad (2.54)$$

where $N_{\uparrow\downarrow}$ represents the number of particles in a defined spin state, and $n_{\uparrow\downarrow}$ represents the relative occupation number of a spin state (up or down).

In a weak magnetic field $B \ll B_C^H$ in the so-called Zeeman region, due to strong spin coupling, the mixed states $|2\rangle$ and $|4\rangle$ do not contribute to the polarization. The polarized gas target for the PAX Spin-Filter experiment will be operated in a weak field. The polarized gas target will consist of state $|1\rangle$ only (see Sec. 5).

2.3.2. Deuterium Polarization

The deuterium polarization is calculated similar to the hydrogen case and is given by:

$$P_e = \sum_{i=1}^6 \langle i | \frac{2}{\hbar} S_z | i \rangle = n_1 - n_4 + (n_2 - n_6) \cos 2\theta_+ + (n_3 - n_5) \cos 2\theta_- \quad (2.55)$$

$$P_z = \sum_{i=1}^6 \langle i | \frac{2}{\hbar} I_z | i \rangle = n_1 + n_6 - n_3 - n_4 + (n_2 - n_6) \sin^2 \theta_+ + (n_3 - n_5) \sin^2 \theta_-. \quad (2.56)$$

Since the deuteron has three spin states $m_I = 1, 0, -1$, an additional tensor polarization P_{zz} is required to fully describe the spin state. P_{zz} is the $z - z$ component of the tensor operator $I_{ij} = \frac{3}{2}(I_i I_j + I_j I_i)$ [77, 70]

$$P_{zz} = \langle I_{zz} \rangle = \langle 3I_z^2 - 2 \rangle, \quad (2.57)$$

and using the basis of Table 2.2:

$$P_{zz} = n_1 + n_4 - \frac{1}{2}(n_2 + n_3 + n_5 + n_6) - \frac{3}{2}(n_2 - n_6) \cos 2\theta_+ + \frac{3}{2}(n_3 - n_5) \cos 2\theta_-. \quad (2.58)$$

The mixing coefficients $\theta_{\pm}$ (Table 2.1, Fig. C.2) are used to define the polarization in (2.55)-2.58. The expectation values of the polarization P_e , P_z and P_{zz} as function of the magnetic field are shown in Fig. 2.3.

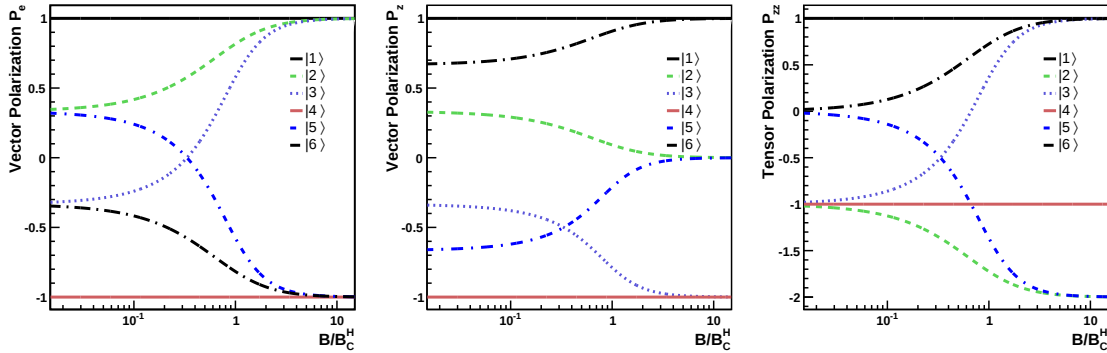


Fig. 2.3.: Expectation values for the polarization of the respective hyperfine states of deuterium. The pure states $|1\rangle$ and $|4\rangle$ are independent of the magnetic field.

2.4. Hyperfine Transitions

Transitions between the hyperfine energy levels are important in the polarization generation and its measurement as well as for the depolarization due to wall collisions or spin-exchange collisions inside the storage cell.

In Sec. 2.2 the solution for the static Hamiltonian (2.28) is achieved with the orthogonal transformation U_0 (2.42). This transformation is now used to analyze the non-static behavior of the hyperfine structure.⁴ Applying the Schrödinger equation to the states of Table 2.2,

$$i\hbar\dot{\Psi} = \mathcal{H}\Psi, \quad (2.59)$$

this equation can be transformed by the orthogonal operator U_0 into

$$i\hbar(\dot{U}_0^T \Psi + U_0^T \dot{\Psi}) = (U_0^T \mathcal{H} U_0 + i\hbar \dot{U}_0^T U_0) U_0^T \Psi. \quad (2.60)$$

Using the new basis $\chi = U_0^T \Psi$, (2.60) can be expressed as

$$i\hbar\dot{\chi} = (\mathcal{H}_{diag}^{st} + i\hbar \dot{U}_0^T U_0) \chi, \quad (2.61)$$

where $\mathcal{H}_{diag}^{st}$ is the static Hamiltonian from the transformation (2.41). For a magnetic field constant in time, the term $\dot{U}_0^T U_0$ vanishes and the eigenstates in Table 2.3 are the eigenstates of $\mathcal{H}_{diag}^{st}$ as calculated before. However, if the magnetic field is time-dependent, the term $\dot{U}_0^T U_0$ induces a distortion of the eigenstates which can result in a transition between two states.

⁴A detailed analysis of the hyperfine transitions is found in [71, 70].

A transition between two states $|a\rangle$ and $|b\rangle$ can be achieved with photons of a specific frequency corresponding to the energy difference $E_a - E_b$, which depends on the static magnetic field:

$$\nu_{ab} = \frac{|E_a - E_b|}{2\pi\hbar} \quad (2.62)$$

Transitions are classified according to the total spin difference and the orientation of the time-dependent magnetic field. A transition induced with the time-dependent magnetic field parallel to the static field is called a σ transition and a perpendicular orientation induces a π transition.

2.4.1. Hyperfine σ Transition

A magnetic field $B(t)$ oscillating parallel to the static field B_z^{st} along the z-axis is given by:

$$\mathbf{B} = (0, 0, B_z^{st} + B(t)). \quad (2.63)$$

With $B(t) = B_{\parallel} \cos \omega t$, $c = \cos \theta$, and $s = \sin \theta$ the time-dependent Hamiltonian (2.61)

$$\{\mathcal{H}_1^{\sigma}\}_{ab} = \{i\hbar \dot{U}_0^T U_0\}_{ab} \quad (2.64)$$

becomes⁵

$$\mathcal{H}_1^{\sigma} = i\hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & s\dot{s} + c\dot{c} & 0 & -s\dot{c} + c\dot{s} \\ 0 & 0 & 0 & 0 \\ 0 & s\dot{c} - c\dot{s} & 0 & s\dot{s} + c\dot{c} \end{pmatrix} = \frac{i\hbar\nu}{2} \frac{B_{\parallel}}{B_C^H} \sin \omega t \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sin^2 \theta \\ 0 & 0 & 0 & 0 \\ 0 & -\sin^2 \theta & 0 & 0 \end{pmatrix}. \quad (2.65)$$

For hydrogen, according to (2.65), the σ transition can only induce a transition between the states $|2\rangle$ and $|4\rangle$ with $\Delta F = \pm 1$, $\Delta m_F = 0$:

$$\sigma|2\rangle \leftrightarrow |4\rangle$$

For deuterium the two possible σ transitions are $\sigma|2\rangle \leftrightarrow |6\rangle$ and $\sigma|3\rangle \leftrightarrow |5\rangle$.

2.4.2. Hyperfine π Transition

For a π transition the time-dependent magnetic field is perpendicular to the static field and can be aligned along either the x or y axis. The Hamiltonian (2.28) in the basis (2.34) is decomposed in a static part and a transition part:

$$\mathcal{H}_{HFSz} = \mathcal{H}_0^{st} + \mathcal{H}_0^{\pi}. \quad (2.66)$$

In the Breit-Rabi basis (Table 2.2) with (2.41), the Hamiltonian $\mathcal{H}_0^{st}$ is transformed into:

$$\mathcal{H}_1^{\pi} = U_0^T \mathcal{H}_0^{\pi} U_0. \quad (2.67)$$

With the time-dependent magnetic field oscillation $B(t)$ in the x axis:

$$\mathbf{B} = (B(t), 0, B_z^{st}), \text{ and } B(t) = B_{\perp} \cos \omega t, \quad (2.68)$$

the transition Hamiltonian transforms into

$$\mathcal{H}_1^{\pi} = \frac{i\hbar\nu}{2} \frac{B_{\perp}}{B_C^H} \cos \omega t \begin{pmatrix} 0 & \sin \theta & 0 & -\cos \theta \\ \sin \theta & 0 & -\cos \theta & 0 \\ 0 & \cos \theta & 0 & -\sin \theta \\ \cos \theta & 0 & -\sin \theta & 0 \end{pmatrix}. \quad (2.69)$$

⁵The index 1 denotes the representation of the Hamiltonian in the Breit-Rabi basis of Table 2.2.

Consequently, a high-frequency magnetic field perpendicular to the static field can induce the following transitions with $\Delta m_F = \pm 1$:

$$\pi|1\rangle \leftrightarrow |2\rangle; \pi|2\rangle \leftrightarrow |3\rangle; \pi|1\rangle \leftrightarrow |4\rangle; \pi|3\rangle \leftrightarrow |4\rangle.$$

A summary and classification of the possible hyperfine transitions for hydrogen and deuterium are given in Table 2.4. Transitions with $\Delta F = 1$ are called SFT for *Strong Field Transition* and transitions with $\Delta F = 0$ are called WFT or MFT for *Weak- and Medium Field Transition*[78, 79, 80, 81, 82].

Table 2.4.: Classification of hydrogen and deuterium hyperfine transitions.

B orientation	σ/π	Type	ΔF	Δm_F	Hydrogen	Deuterium
$B_{HF} \parallel B_z$	σ	SFT	1	0	$2 \leftrightarrow 4$	$2 \leftrightarrow 6, 3 \leftrightarrow 5$
$B_{HF} \perp B_z$	π	SFT	1	1	$1 \leftrightarrow 4$ $3 \leftrightarrow 4$	$1 \leftrightarrow 6, 2 \leftrightarrow 5$ $3 \leftrightarrow 6, 4 \leftrightarrow 5$
$B_{HF} \perp B_z$	π	MFT	0	1	$1 \leftrightarrow 2$ $2 \leftrightarrow 3$	$1 \leftrightarrow 2, 2 \leftrightarrow 3$ $5 \leftrightarrow 6, 3 \leftrightarrow 4$

2.4.3. Adiabatic High-Frequency Transitions

An atom subjected to the transition resonance will oscillate between the transition states $|a\rangle$ and $|b\rangle$. A selective transition is only possible if the time for which the atom experiences the resonance perfectly matches the transition time[83]. This condition is not possible for an atomic beam with a thermal velocity distribution in a constant magnetic field. The so-called *adiabatic transition* superimposes a gradient magnetic field to the static magnetic field along the path of the atoms. The gradient assures that the atoms will experience the transition condition only once.

The Atomic Beam Source (ABS) and the Breit-Rabi Polarimeter (BRP) make use of adiabatic high-frequency transitions to exchange hyperfine state populations. The central aspect of the adiabatic transition is that two hyperfine populations are fully exchanged, in practice efficiencies close to 100% can be achieved. The function principle is based on the interaction of the atomic beam with a high-frequency electromagnetic field and a static magnetic field as described in Sec. 2.4.1 and Sec. 2.4.2. The quantum mechanical explanation follows [84, 85].

For simplicity only a two states system as encountered in spin 1/2 particles is discussed (for more details see [71]). The corresponding energies E_1 and E_2 of the states $|1\rangle$ and $|2\rangle$ depend on the magnetic field as seen in Sec. 2.2 and are schematically plotted in Fig. 2.4a. The addition of a time-dependent magnetic field is treated as a perturbation:

$$\mathcal{H}_{ad} = \mathcal{H}^{st} + \mathcal{H}^{rot} \quad \text{with} \quad \mathcal{H}^{rot} = i\hbar \dot{U}_0^T U_0 \quad (2.70)$$

as seen in (2.64). The time-dependent magnetic field term $i\hbar \dot{U}_0^T U_0$ in the co-rotating frame is no longer diagonal (2.65) and causes a shift of the energies; it is illustrated in Fig. 2.4b. When the perturbed Hamiltonian is diagonalized, the eigenstates are separated (Fig. 2.4c); they can be described as a linear combination of the initial unperturbed static states:

$$\begin{aligned} |a\rangle &= \cos \phi |1\rangle + \sin \phi |2\rangle \\ |b\rangle &= \sin \phi |1\rangle + \cos \phi |2\rangle \end{aligned} \quad (2.71)$$

This means that in the rotating frame, due to the high-frequency term, the co-rotating eigenstates $|a\rangle$ and $|b\rangle$ are now a mixture of the static states $|1\rangle$ and $|2\rangle$. The mixing angle ϕ depends on the static field B and the high-frequency field amplitude. The eigenstates $|a\rangle$ and $|b\rangle$ are so-called *adiabatic*

eigenstates and are separated by an energy barrier. The movement of an atom through the transition along a positive gradient is equivalent to passing from left to right in the Breit-Rabi diagram 2.4c⁶. As long as the atom stays in its adiabatic eigenstate composed of $|1\rangle$ and $|2\rangle$, the atom will enter as state $|2\rangle$ (or $|1\rangle$) and leave the transition as state $|1\rangle$ (or $|2\rangle$).

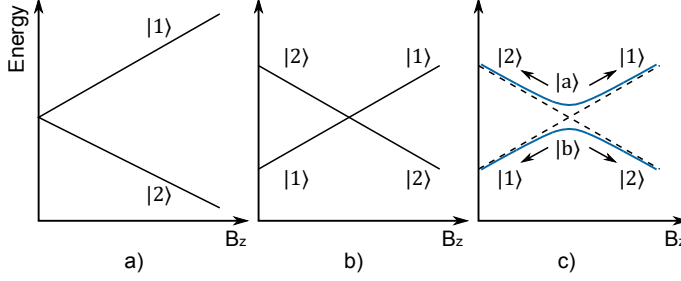


Fig. 2.4.: Visualization of the quantum mechanical treatment of the adiabatic transition [84]. a) A schematic view of the Breit-Rabi diagram for two states. b) The high-frequency term in the Hamiltonian lowers or raises the energies. c) A high rf amplitude separates the two states and creates a gap at the cross point.

If the frequency amplitude is not large enough or the passage through the field happens too fast, the energy barrier between the two co-rotating states is reduced and the atom can keep its original state by migrating to the other adiabatic eigenstate. The transition probability is given by: [84]

$$p = e^{-2\pi\kappa} \text{ with } \kappa = \left| \frac{\mu_j B_{HF}^2}{2\hbar\dot{B}} \right|. \quad (2.72)$$

A high transition probability requires $\kappa \gg 1$ leading to the adiabatic condition

$$\mu_j B_{HF}^2 \gg 2\hbar\dot{B}. \quad (2.73)$$

Experimentally this means that the amplitude of the rf-field must be as large as possible. The experimental MFT and SFT transition conditions for hydrogen and deuterium are shown in Fig. 2.5.

The SFTs are single photon transitions and the magnetic field strength between different transitions is well separated compared to the MFTs. The experimental resonance identification is therefore simpler. The MFTs are technically also single photon transitions; however, they have up to two (three for deuterium) transitions taking place sequentially. Furthermore, the order of the transition depends on the gradient direction. For example, the transition MFT 1-3 is a transition 1-2 + 2-3 in which case the gradient field must cover both transition conditions within the few cm of the coil. For the MFT 2-3 transition, the gradient must stop before reaching the transition 1-2.

The measurement of the polarization requires the exact knowledge of the efficiencies of all transitions used during the measurement. The effect of a transition on a population of atoms is modeled with a matrix including the transition efficiency. The effect of the transition to the vector of the absolute hyperfine population number $N_a = (N_1, N_2, \dots)^T$ is then given by

$$N_a \longrightarrow \sum_b T_{ab} N_b. \quad (2.74)$$

For example, the transition SFT 1-4 for hydrogen called mode s14, is now modeled using the efficiency ϵ_{s14} :

$$T_{14} = \begin{pmatrix} 1 - \epsilon_{s14} & 0 & 0 & \epsilon_{s14} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \epsilon_{s14} & 0 & 0 & 1 - \epsilon_{s14} \end{pmatrix}. \quad (2.75)$$

⁶The horizontal axis can be interpreted as position or time in a gradient field in the rest frame of the atoms.

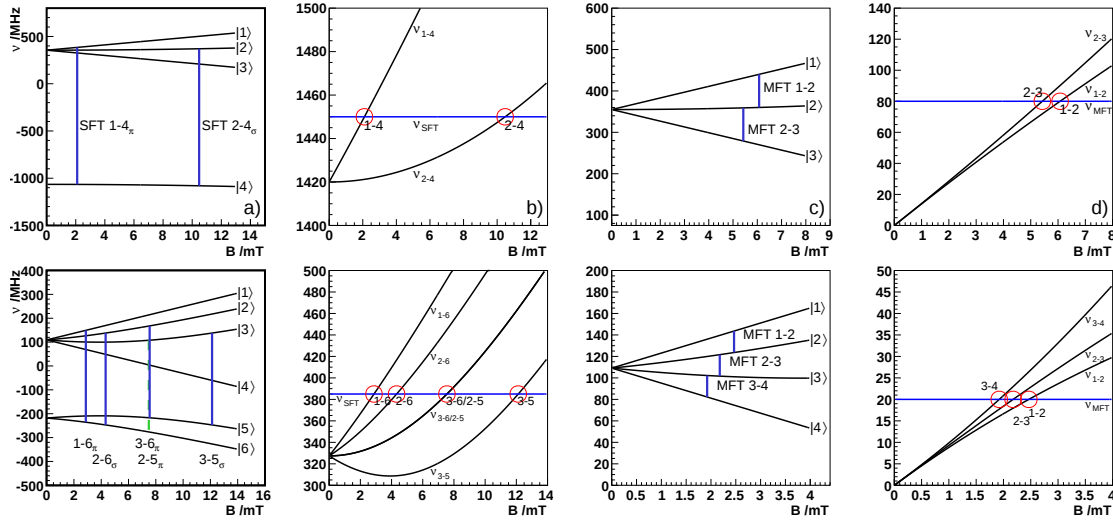


Fig. 2.5.: SFT and MFT transition conditions for hydrogen and deuterium. The top four plots are for hydrogen and the bottom four for deuterium. Plots (a) and (b) show the SFT conditions for an operating frequency of 1450 MHz (385 MHz for deuterium). In plot (a) the frequency value is shown in the Breit-Rabi diagram as a vertical line, in (b) the transition frequencies are the difference between the two corresponding energies of the two states. The magnetic field necessary for the transition is reached when the transition frequency crosses the operating frequency. The same principle applies for the MFT in figures (c) and (d). The transition conditions are marked with a circle. The hydrogen SFT 3-4 is not used as the sextupole magnet removes both states and this transition is thus not useful. The deuterium transitions SFT 3-6 and 2-5 share the same frequency and magnetic field and occur simultaneously.

In the ideal case where $\epsilon_{14} = 1$, the transformation (2.74) for s_{14} becomes

$$\begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \end{pmatrix} \xrightarrow{s_{14}} \begin{pmatrix} N_4 \\ N_2 \\ N_3 \\ N_1 \end{pmatrix}. \quad (2.76)$$

The MFT multiple transitions are modeled with one matrix for each single transition. For example, the MFT 1-3 (mode m_{13}) is given by $T_{13} = T_{12}T_{23}$ with the efficiencies $\epsilon_{m_{12}}$ and $\epsilon_{m_{23}}$. An important difference to the SFT is that all transitions must be considered in the model even if only one is active. For instance, the efficiency $\epsilon_{m_{12}}$ must be included in the single transition MFT 2-3 because a non-zero efficiency is technically unavoidable. The MFT 1-3 transition is thus described by the same model as the MFT 2-3, but with different efficiencies. Furthermore, the gradient direction is reflected by the sequence of the matrix multiplication:

$$T_{13(-)} = T_{23}T_{12} \text{ for a decreasing gradient} \quad (2.77)$$

$$T_{13(+)} = T_{12}T_{23} \text{ for an increasing gradient.} \quad (2.78)$$

Explicitly this leads (with $\epsilon_i = 1$) to

$$T_{13(-)} = \begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \end{pmatrix} \xrightarrow{m_{12}} \begin{pmatrix} N_2 \\ N_1 \\ N_3 \\ N_4 \end{pmatrix} \xrightarrow{m_{23}} \begin{pmatrix} N_2 \\ N_3 \\ N_1 \\ N_4 \end{pmatrix} \neq T_{13(+)} = \begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \end{pmatrix} \xrightarrow{m_{23}} \begin{pmatrix} N_1 \\ N_3 \\ N_2 \\ N_4 \end{pmatrix} \xrightarrow{m_{12}} \begin{pmatrix} N_3 \\ N_1 \\ N_2 \\ N_4 \end{pmatrix}. \quad (2.79)$$

The order of the transitions can be deduced from Fig. 2.5c. It is important to note in Eq. (2.79) that the $T_{13(+)}$ transition will produce the same signal on the Quadrupole Mass Analyzer (QMA) as the T_{23} transition because in both cases the signal after the sextupole magnets is composed of the populations $N_2 + N_4$. The BRP MFT has to use a negative gradient.

2.5. Spin Separation in Sextupole Magnets

The sextupole magnets are used to separate atoms according to their electron spin orientation by making use of the Stern-Gerlach force induced by an inhomogeneous magnetic field. The separation of atoms in an atomic beam based on their magnetic moment produced by the spin was discovered by Stern and Gerlach in 1922 [86, 87]

The deflecting force is derived from the potential energy of the magnetic field[88, 65, 89, 90]:

$$U = -\boldsymbol{\mu}\mathbf{B} = -\mu_B \frac{g_s}{2} B_z \quad (2.80)$$

The force is the negative of the derivative of the potential energy U ; thus, with $g_s \simeq 2$

$$F_z = -\frac{\partial U}{\partial z} = \pm \mu_B \frac{\partial B_z}{\partial z}. \quad (2.81)$$

The deflection is therefore proportional to the magnitude of the magnetic field gradient and to the magnetic moment generated by the spin.

In the experiment the inhomogeneous magnetic field is generated by a permanent sextupole magnet. The magnet is a circular arrangement of 24 permanent magnets made of a NdFeB alloy [91]. Each segment has a magnetization rotated by 60° relative to its neighbor. Figure 2.6 shows the schematic assembly of a sextupole magnet used for spin separation. The magnetic field strength

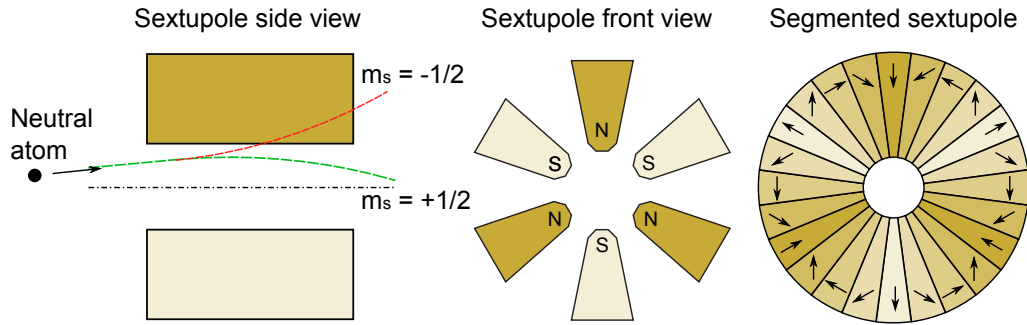


Fig. 2.6.: Sextupole magnet configuration scheme [92]. The central figure shows a typical sextupole arrangement. The permanent magnet sextupole used in the ABS and BRP are constructed with 24 trapezoid segments to create the same magnetic field configuration as in the central figure.

depends quadratically on the distance from the sextupole axis [93, 94]:

$$B(r) = B_{pt} \frac{r^2}{r_{pt}^2}, \quad (2.82)$$

with B_{pt} the maximal field at the pole tip and r_{pt} the pole tip radius. The force acting on the atoms is axial and its direction depends on the spin sign $\pm m_s$ [91]:

$$\vec{F}_{r\pm} = \mp \mu_B 2 \frac{B_{pt}}{r_{pt}^2} \cdot r^2. \quad (2.83)$$

Atoms with negative spin $m_s = -\frac{1}{2}$ are defocused, recombine on the walls and are pumped out of the nominal path. Only atoms with positive spin and having a velocity matching the magnetic optics are focused by the sextupole magnets and are able to exit into the next chamber or detector. Therefore, behind the sextupole system, the atomic beam is fully electron polarized because atoms with negative electron spin have been removed from the beam. This ideal case is only valid for the BRP with a beam blocker, in the ABS some atoms with negative spin are leaking through, e.g., 5% of the prefocused state $|2\rangle$ interchanged to 3 with the MFT reach the cell [95].

Following the same principle as with (2.74), the sextupole effect on the population vector is described by the transmission probabilities σ_i of a state $|i\rangle$ to pass the sextupole.

$$N_a \longrightarrow \sum_b \sigma_b N_b. \quad (2.84)$$

For example, considering the ideal case where $\sigma_1 = \sigma_2 = 1$ and $\sigma_3 = \sigma_4 = 0$, the population vector is transformed as:

$$\sigma \mathbf{N} = (\sigma_1 \ \sigma_2 \ \sigma_3 \ \sigma_4) \begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \end{pmatrix} = \begin{pmatrix} N_1 \\ N_2 \\ 0 \\ 0 \end{pmatrix}. \quad (2.85)$$

3. THEORY OF THE POLARIZATION MEASUREMENT AND CALIBRATION

3.1. Working Principle of the Breit-Rabi Polarimeter

The BRP measures the polarization by determining the relative intensities of all hyperfine states of a sample beam from the storage cell. The polarization is then calculated as described in Sec. 2.3 with Eq. (2.51) for hydrogen and Eqs. (2.55), (2.58) for deuterium.

The three components of the BRP are a set of adiabatic High Frequency Transitions (HFT) discussed in Sec. 2.4.3, two sextupole magnets and a Quadrupole Mass Analyzer (QMA). The QMA is used as a detector to measure the beam intensity. A rotating chopper is installed in front of the QMA to subtract the background. A schematic view of the BRP components is shown in the top part of Fig. 3.1.

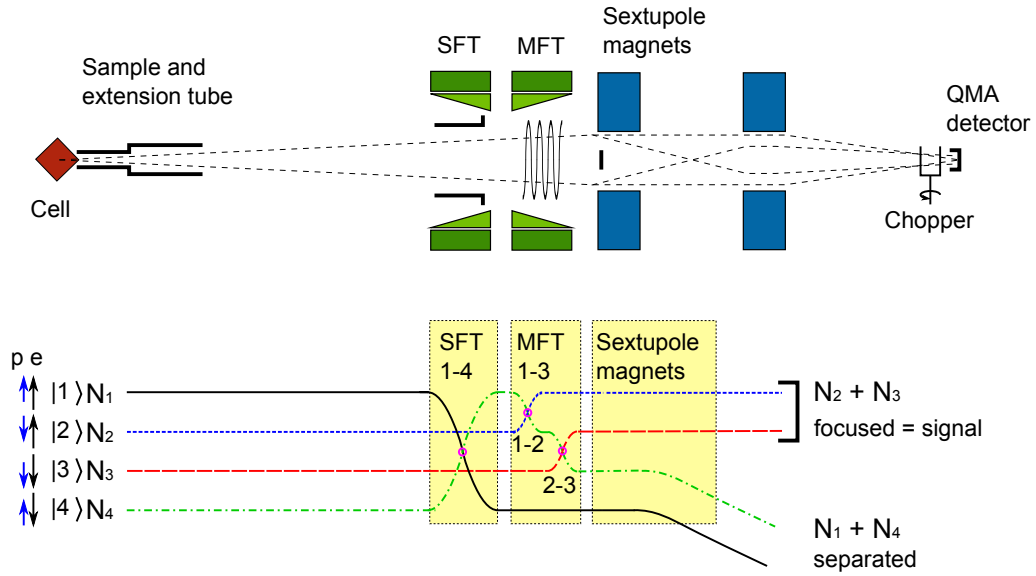


Fig. 3.1.: On top: schematic view of the BRP components. On bottom: signal example with transitions SFT_{14} and MFT_{13} with decreasing gradient switched on. The transition SFT_{14} exchanges the populations $N|1\rangle \leftrightarrow N|4\rangle$ while the MFT_{13} is a double transition. First the populations $N|1\rangle \leftrightarrow N|2\rangle$ are exchanged then followed by $N|2\rangle \leftrightarrow N|3\rangle$. The sextupole magnets thus remove the initial state populations $N|1\rangle$ and $N|4\rangle$ and focus the initial state populations $N|2\rangle$ and $N|3\rangle$ into the detector.

In a first step the HFTs exchange two or more hyperfine state populations. The following sextupole magnets act as a spin filter and separates the atoms based on their electron spin. The atoms with spin $m_s = -\frac{1}{2}$, effectively the final states $|3\rangle$ and $|4\rangle$ after the HFTs, are removed from the beam while the atoms with spin $m_s = +\frac{1}{2}$ are focused into the QMA. The beam blocker ensures that none of the states $|3\rangle$ or $|4\rangle$ reaches the QMA (see Sec. 4.4.3).

The combination of hyperfine state population exchange and sextupole filter permits one to select different initial hyperfine state combinations. In the ideal case this results in a signal composed of two different initial states as illustrated in the lower Fig. 3.1. By switching a transition on or off, the

hyperfine states behind the sextupole magnets will be differently occupied. The detector measures a signal proportional to the sum of the hyperfine populations with $m_s = +\frac{1}{2}$; the signal will vary based on the HFT mode and the target gas polarization.

Different combinations of HFT modes are sequenced in such a way as to measure all relative occupation numbers n_i . The polarization is then determined with Eq. (2.51). The theoretical framework to measure the polarization and determine the statistical and systematic errors is presented in the next section.

3.2. Theory of the Polarization Measurement

The measured BRP signals are a linear combination of the four hyperfine state intensities I_a . Each intensity is proportional to the sum of populations N_a in the state $|a\rangle$. For example, for hydrogen there are 11 different signal combinations S_i based on different HFTs modes. The signals are modeled as [71]:

$$S_i = \sum_a M_{ia} I_a; \quad \text{with} \quad M_{ia} = \sum_b \sigma_b \prod_j T_{ba}^j. \quad (3.1)$$

The so-called *measurement matrix* M_{ia} describes the physical effect of the transitions T_{ba}^j (2.74) and the sextupole magnets σ_b (2.85). The transition matrix T_{ba}^j includes the efficiencies of the transitions and the vector σ_b contains the sextupole transmission probabilities. For example, the signal with all transitions off is reduced to

$$S_{\text{rft off}} = \sum_a \sigma_a I_a \quad (\text{see Eq. (2.85)}), \quad (3.2)$$

while a measurement signal with the transition SFT₂₄ in operation is given by

$$S_{s24} = \sum_a M_{24,a} I_a = \sum_a \sigma_a T_{24} I_a \quad (3.3)$$

$$S_{s24} = I_1 \sigma_1 + I_3 \sigma_3 + I_4 (\sigma_4 (1 \epsilon_{s24}) + \sigma_2 \epsilon_{s24}) + I_2 (\sigma_2 (1 \epsilon_{s24}) + \sigma_4 \epsilon_{s24}). \quad (3.4)$$

The product $\prod_j T^j$ takes into account the fact that more than one transition is active or as in the MFT case that two transitions occur sequentially. For example, the signal S_{s14m13} seen in Fig. 3.1 using the transitions SFT₁₄ and MFT₁₃ is described with

$$S_{s14m13} = \sum_a \sigma_a T_{23} T_{12} T_{14} I_a, \quad (3.5)$$

this leads explicitly to

$$\begin{aligned} S_{s14m13} = & I_4 [\sigma_4 (1 - \epsilon_{s14}) + \sigma_1 \epsilon_{s14}] + \\ & + I_1 [\epsilon_{m12} \sigma_2 + (1 - \epsilon_{m12}) (\sigma_1 (1 - \epsilon_{s14}) + \sigma_4 \epsilon_{s14})] + \\ & + I_2 [\epsilon_{m23} \sigma_3 + (1 - \epsilon_{m23}) ((1 - \epsilon_{m12}) \sigma_2 + \epsilon_{m12} (\sigma_1 (1 - \epsilon_{s14}) + \sigma_4 \epsilon_{s14}))] + \\ & + I_3 [(1 - \epsilon_{m23}) \sigma_3 + \epsilon_{m23} ((1 - \epsilon_{m12}) \sigma_2 + \epsilon_{m12} (\sigma_1 (1 - \epsilon_{s14}) + \sigma_4 \epsilon_{s14}))]. \end{aligned}$$

The solution for the unknown intensities I_a for i signals in (3.1) is given by

$$I_a = \sum_i R_{ai} S_i, \quad (3.6)$$

with R being the inverse measurement matrix $R_{ai} = M_{ia}^{-1}$. This Eq. (3.6) can be solved if the measurement matrix $\mathbf{M}$ is known. The transition efficiencies ϵ_i and transmission probabilities of the sextupoles σ_j entering the measurement matrix are measured in the calibration procedure described in Sec. 3.3.

A better statistical accuracy is reached by collecting more signals than unknowns to achieve an overdetermined system. In this case R is the *pseudo-inverse* matrix of $\mathbf{M}$:

$$\mathbf{R} = (\mathbf{M}^T \mathbf{W}_S \mathbf{M})^{-1} \mathbf{M}^T \mathbf{W}_S. \quad (3.7)$$

The weighting matrix $\mathbf{W}_S$ is the inverse covariance matrix (3.15) of the measured signals. Eq. (3.7) is equivalent to a least square fit. The solution for the intensities is calculated with the normal equation [96, 97]

$$\mathbf{I} = (\mathbf{M}^T \mathbf{W}_S \mathbf{M})^{-1} \mathbf{M}^T \mathbf{W}_S \mathbf{S} \quad (3.8)$$

with $\mathbf{S}$ the vector of measured signals. The total intensity is given by the sum of all hyperfine states

$$I_{tot} = \sum_a I_a, \quad (3.9)$$

and the relative hyperfine populations n_a . Necessary for the polarization measurement are the intensities normalized with the total intensity:

$$n_a = \frac{I_a}{I_{tot}}. \quad (3.10)$$

The polarization does not only depend on the individual relative hyperfine state populations n_a but also, as seen in Sec. 2.3, on the mixing angle θ which impacts the mixing of the states. The polarization contribution of the mixed hyperfine states depends on the target magnetic holding field B and is described by the matrices

$$\mathbf{M}_P^H = \begin{pmatrix} 1 & \cos 2\theta & 1 & -\cos 2\theta \\ 1 & -\cos 2\theta & -1 & \cos 2\theta \end{pmatrix} \quad \text{and} \quad (3.11)$$

$$\mathbf{M}_P^D = \begin{pmatrix} 1 & C_+ & C_- & -1 & -C_- & -C_+ \\ 1 & \sin^2 \theta_+ & -\cos^2 \theta_- & -1 & -\sin^2 \theta_- & \cos^2 \theta_+ \\ 1 & -\frac{1}{2}(3C_+ + 1) & \frac{1}{2}(3C_- - 1) & 1 & -\frac{1}{2}(3C_- + 1) & \frac{1}{2}(3C_+ - 1) \end{pmatrix}, \quad (3.12)$$

with $C_{\pm} = \cos 2\theta_{\pm}$. The mixing angle θ depends on the magnetic field (Table 2.1). The matrices $\mathbf{M}_P^{H,D}$ are the matrix representation of Eqs. (2.51),(2.52) and (2.55),(2.58). Using the mixing matrices (3.11), the hydrogen and deuterium nuclear and electron polarization can now be expressed in a matrix notation:

$$(P_e, P_z)^T = \mathbf{M}_P^H(n_1, n_2, n_3, n_4)^T \quad (3.13)$$

$$(P_e, P_z, P_{zz})^T = \mathbf{M}_P^D(n_1, n_2, n_3, n_4, n_5, n_6)^T. \quad (3.14)$$

3.2.1. Statistical Uncertainty of the Polarization Measurement

The signals S_i being independent measurements, the variation δ_i^2 of each signal can be arranged into a diagonal covariance matrix $\mathbf{C}_S$ of the signals¹:

$$\mathbf{C}_S = \begin{pmatrix} \delta_1^2 & & 0 \\ & \delta_2^2 & \\ 0 & & \ddots \\ & & & \delta_n^2 \end{pmatrix}. \quad (3.15)$$

The weighting matrix of the signals is defined as $\mathbf{W}_S = \mathbf{C}_S^{-1}$. The covariance matrix of the calculated intensities is defined as [98]

$$\mathbf{C}_I = (\mathbf{R} \mathbf{C}_S \mathbf{R}^T) = (\mathbf{M}^T \mathbf{W}_S \mathbf{M})^{-1}. \quad (3.16)$$

¹To avoid confusion with the sextupole transmission probabilities σ , the variation is call δ^2 instead of σ^2 .

The elements of the covariance matrix $\mathbf{C}_n$ of the relative hyperfine populations are calculated with error propagation as

$$(C_n)_{a,b} = \sum_{c,d} \left(\frac{\partial n_a}{\partial I_c} \right) (C_I)_{c,d} \left(\frac{\partial n_b}{\partial I_d} \right). \quad (3.17)$$

The covariance matrix of the polarization vectors for hydrogen and deuterium is given by

$$\mathbf{C}_P = \mathbf{M}_P^{\text{H,D}} \mathbf{C}_n (\mathbf{M}_P^{\text{H,D}})^T. \quad (3.18)$$

The statistical error i^{th} of the polarization vector is extracted from the covariance matrix (3.18):

$$\delta_{P_i, \text{stat}} = \sqrt{\chi^2(I) C_{Pii}}. \quad (3.19)$$

The $\chi^2(I)$ quality of fit for the intensities is the weighted sum of the residuals between the signals S_i and the model $F(\epsilon_j, \sigma_k, I_l) = \sum_a M_{ia} I_a$:

$$\chi_{\text{fit}}^2 = \sum_{i=1}^m \left[\frac{S_i - F(\epsilon_j, \sigma_k, I_l)}{\delta_i} \right]^2. \quad (3.20)$$

Combining the signals and the model into vectors, the residual vector is defined as

$$\mathbf{K} = \mathbf{S} - \mathbf{F}(\epsilon_j, \sigma_k, I_l), \quad (3.21)$$

and the $\chi^2(I)$ per degree of freedom² can be expressed using the vector notation:

$$\chi^2(I) = \frac{\mathbf{K}^T \mathbf{W}_s \mathbf{K}}{r}. \quad (3.22)$$

The degree of freedom $r = i - a$ is the difference between i equations (signals) and a unknown intensities. The statistical error depends on both the quality of the fit and the errors on the measured signals.

3.2.2. Systematic Uncertainty of the Polarization Measurement

The systematic uncertainty of the polarization depends on the covariance of the calibration efficiencies $\mathbf{C}_\epsilon$. The covariance together with the quality of the fit χ^2 represents the statistical uncertainty of the calibration parameters and is obtained with the calibration algorithm (Sec. 3.3). The systematic error of the intensities depends on the statistical error of the efficiencies, it is given by [71]:

$$\mathbf{C}_{\mathbf{I}, \text{sys}} = \mathbf{T}_\epsilon \mathbf{C}_\epsilon \mathbf{T}_\epsilon^T. \quad (3.23)$$

The matrix $\mathbf{T}_\epsilon$ relates the dependence of the intensities I_k to the transition efficiencies ϵ_l with

$$(T_\epsilon)_{k,l} = \left(\frac{\partial I_k}{\partial \epsilon_l} \right) = \sum_j \left(\frac{\partial I_k}{\partial S_j} \right) \cdot \left(\frac{\partial S_j}{\partial \epsilon_l} \right). \quad (3.24)$$

The first matrix in (3.24) is identical to the matrix $\mathbf{R}$ (3.7):

$$R_{kj} = \frac{\partial I_k}{\partial S_j}. \quad (3.25)$$

The second matrix in (3.24) describes the dependence of the signals towards the efficiencies. It can be calculated with the partial derivate according to each efficiency or directly from the measurement matrix (3.1):

$$\frac{\partial S_j}{\partial \epsilon_l} = \sum_k [M_{jk}(\epsilon_1, \dots, \epsilon_l + 1, \dots, \epsilon_n) - M_{jk}(\epsilon_1, \dots, \epsilon_l, \dots, \epsilon_n)] \cdot I_k. \quad (3.26)$$

²The value $\chi^2(I)$ is the χ^2 quality of the fit for the intensities $\mathbf{I}$.

The direct method is possible because each efficiency enters linearly into $\mathbf{M}$. The propagation of the systematic errors from the covariance matrix $\mathbf{C}_{\mathbf{I},\text{sys}}$ are extracted using (3.16) to (3.18) leading to the standard systematic error

$$\delta_{Pi,\text{sys}} = \sqrt{\chi^2(\epsilon) C_{Pii}(\text{sys})}. \quad (3.27)$$

The $\chi^2(\epsilon)$ is the quality of the fit for the calibration of the BRP.

3.3. Theory of the Calibration

The polarization of the atomic beam can be calculated provided the so-called measurement matrix M_{ia} is known. The procedure to measure the transition efficiencies and transmission probabilities and thus to determine the matrix M_{ia} is called the BRP calibration.

As shown in Sec. 3.2 each row i of the matrix M_{ia} corresponds to the effect of a specific setting of the transitions and leads to the description of the signal generated by this mode. For example, the signal S_{s14m13} generated by selecting the transition $\text{SFT}_{14} + \text{MFT}_{13}$ is described by the row $M_{s14m13,a}$ of the measurement matrix. Supposing all efficiencies and transmission probabilities are ideally either 0 or 1, this leads to the row vector:

$$M_{s14m13,a} = \boldsymbol{\sigma} \cdot T_{23} T_{12} T_{14} = (0 \quad 1 \quad 1 \quad 0). \quad (3.28)$$

With Eq. (3.1), the corresponding signal is

$$S_{s14m13} = \sum_a M_{s14m13,a} \cdot I_a = I_2 + I_3 \quad (3.29)$$

as demonstrated schematically in Fig. 3.1.

The principle of the calibration is to generate and measure enough different signal combinations to ensure that Eq. (3.1) is overdetermined. The unknown efficiencies are indirectly extracted by fitting the model (3.1) to the acquired data.

All possible transition combinations including magnetic cross-talk (as explained in Sec. 5.1.1) lead to 11 different signals for hydrogen. The modes and efficiencies configuration in respect to the experimental setup is described in detail in Sec. 5. For the polarization this overdetermined linear system of 11 signals and 4 unknown intensities can be solved with a least square fit algorithm. However, for the calibration both the efficiencies including the sextupole transmission probabilities as well as the intensities are unknown, leading to an underdetermined system of equations. This problem is solved by injecting different modes from the ABS into the storage cell. In this case the total number of collected signals is $N_s = N_{\text{ABS}} \cdot N_{\text{BRP}}$ with N_{ABS} injection modes and N_{BRP} measurement modes. The number of unknown is $N_u = N_{\text{eff}} + N_{\text{ABS}} \cdot N_{\text{HFS}}$ with N_{eff} the unknown calibration parameters of the BRP and N_{HFS} the number of hyperfine states (4 for hydrogen and 6 for deuterium). The system can be solved if the degree of freedom N_f is greater than zero:

$$N_f = N_s - N_u = (N_{\text{BRP}} - N_{\text{HFS}})N_{\text{ABS}} - N_{\text{eff}} \geq 0. \quad (3.30)$$

For example, for hydrogen each ABS injection mode adds 4 new unknown intensities $\mathbf{I}$ and 11 more N_{BRP} signals; however, the number of unknown BRP parameters N_{eff} remains unchanged independent of the cell content. Therefore, each new injected mode effectively adds 7 additional signals to the model (3.1). Table 3.1 gives a comparison of signals and unknowns for 1 and 3 ABS injection modes for hydrogen and deuterium. The minimum required to solve the system of unknowns is 3 different ABS modes, this is also the maximum possible with the single MFT transition installed. The ABS injection modes are $|1\rangle + |2\rangle$, $|2\rangle$ and $|1\rangle$ by selecting the MFT modes *off*, *m23+m12* and *m23* respectively.

The two fitting algorithms which are implemented in the BRP calibration and used to solve Eq. (3.1) are based on standard least square fit methods.

Table 3.1.: Hydrogen and deuterium unknown variables for the calibration. Details of the modes and unknowns are discussed in Sec. 5.

Using 1 ABS mode		Using 3 ABS modes	
H signals	11	H signals	33
H unknown	$10 + 1 + 4 = 15$	H unknown	$11 + 3 \cdot 4 = 23$
D signals	29	D signals	87
D unknown	$40 + 2 + 6 = 48$	D unknown	$42 + 3 \cdot 6 = 60$

3.4. Fitting Algorithm

The calibration procedure and the polarization measurement are both indirect methods. The searched parameters are extracted from the data with a fitting algorithm. The system of equations of the polarization measurement can be solved directly as shown in (3.8); however, the BRP calibration requires to determine both the variables for M_{ia} and I_a in (3.1) at the same time. This nonlinear system of equations must be solved with an iterative algorithm. The two methods used for the BRP calibration are the *Gauss-Newton algorithm* and the *Lagrange multipliers* algorithm.

3.4.1. Least Square Approximation

A system of m measurements x_i of the variable y_i have an error δ_i . A typical non-linear least square problem is to find the simultaneous roots of a system of m equations with n unknown parameters [99], with $m \geq n$. That is, the degree of freedom must be greater than zero; thus, the number of measurements must be greater than the number of unknown parameters³. The system is described by

$$f_i(x; \beta_1, \beta_2, \dots, \beta_n) = 0; \quad i = 1, \dots, m. \quad (3.31)$$

The model functions $g(x_i)$ which describe the measured points y_i depend on the independent variable x and the constrained parameter n -vector of unknown $\beta = (\beta_1, \dots, \beta_n)$. The functions are defined as

$$y_i = g(x_i, \beta). \quad (3.32)$$

The residuals are the difference between the model functions and the data [102]

$$r_i = y_i - g(x_i, \beta); \quad i = 1, \dots, m. \quad (3.33)$$

Here the initial problem to be solved is defined as $f_i(x, \beta) = r_i$. The least square method finds the best values for the vector of unknown β by minimizing the weighted sum of residuals:

$$S = \sum_{i=1}^m \left[\frac{y_i - g(x_i, \beta)}{\delta_i} \right]^2 = \sum_{i=1}^m \left[\frac{r_i}{\delta_i} \right]^2. \quad (3.34)$$

The minimum of (3.34) for the n parameters of β is found when the gradient of S is zero; that is, (and ignoring the errors for now):

$$\frac{\partial S}{\partial \beta_j} = 2 \sum_{i=1}^m r_i \frac{\partial r_i}{\partial \beta_j} = 0. \quad (3.35)$$

This indirect and nonlinear problem can be linearized by using the first Taylor expansion of the model function around the vector β^k of the k th iteration:

$$g(x_i, \beta) = g(x_i, \beta^k) + \sum_j \frac{\partial g(x_i, \beta^k)}{\partial \beta_j} (\beta_j - \beta_j^k) + O^2(\beta_j). \quad (3.36)$$

³See [100] chapter 2, [96] chapter 9 and [101, 97, 102, 103, 104].

With the Jacobi matrix of the model

$$J_{ij} = \frac{\partial g_i}{\partial \beta_j}, \quad (3.37)$$

the Taylor expansion without the higher terms can be written as

$$g(x_i, \boldsymbol{\beta}) = g(x_i, \boldsymbol{\beta}^k) + \sum_j J_{ij} \Delta \beta_j. \quad (3.38)$$

The residuum Eq. (3.33) thus becomes

$$r_i = y_i - g(x_i, \boldsymbol{\beta}^k) + \sum_j J_{ij} \Delta \beta_j. \quad (3.39)$$

Using the residual difference $\Delta y_i = y_i - g(x_i, \boldsymbol{\beta}^k)$ and the Jacobian definition (3.37), the gradient Eq. (3.35) can be rewritten as

$$2 \sum_{i=1}^m J_{ik} \left(\Delta y_i - \sum_{j=1}^n J_{ij} \Delta \beta_j \right) = 0. \quad (3.40)$$

This normal equation is a system of n linear equations:

$$\sum_{i=1}^m \sum_{j=1}^n J_{ik} J_{ij} \Delta \beta_j = \sum_{i=1}^m J_{ik} \Delta y_i; \quad (k = 1, \dots, n) \quad (3.41)$$

and is used to solve linear least square problems. It is usually written in matrix notation:

$$(\mathbf{J}^T \mathbf{J}) \Delta \boldsymbol{\beta} = \mathbf{J}^T \Delta \mathbf{y}. \quad (3.42)$$

Because the measurements do have an error, the weighted sum of the squared residuals has to be calculated with Eq. (3.34). The weight matrix $\mathbf{W}_y$ is the inverse of the covariance matrix $\mathbf{C}_y$ of the measurements: $\mathbf{C}_y = \mathbf{W}_y^{-1}$. The normal equation then becomes

$$(\mathbf{J}^T \mathbf{W} \mathbf{J}) \Delta \boldsymbol{\beta} = \mathbf{J}^T \mathbf{W} \Delta \mathbf{y}. \quad (3.43)$$

The covariance matrix $\mathbf{C}_\beta$ of the fitted parameters is then defined as

$$\mathbf{C}_\beta = (\mathbf{J}^T \mathbf{W} \mathbf{J})^{-1}. \quad (3.44)$$

Equation (3.43) can be solved directly for $\Delta \boldsymbol{\beta}$ with an inverse matrix calculation and constitutes one iteration.

3.4.2. Gauss-Newton iteration

The Jacobi matrix J_{ij} depends on both the observations and unknown parameters; therefore, initial guess values for the parameters must be provided for the first iteration. The normal equation (3.43) is used to solve the *improvement of the parameters* $\Delta \boldsymbol{\beta}$ of the actual residuals $\Delta \mathbf{y}$. The calculation of (3.43) using a matrix inversion is implemented with an LU-decomposition algorithm with full pivoting[99]. The full pivoting method interchanges both rows and columns of the matrix in order to divide by the largest element and therefore reduce numerical rounding errors. The unknown parameters $\boldsymbol{\beta}$ are then improved on each iteration with

$$\boldsymbol{\beta}^{k+1} = \boldsymbol{\beta}^k + \Delta \boldsymbol{\beta}. \quad (3.45)$$

The initial values for the parameters β are the ideal values of the BRP transitions. The improved result refines the parameters on every iteration, the goal being to find the root or local minimum of (3.33). The quality of the fit χ^2 is calculated after each iteration i :

$$\chi^2(i) = \frac{\Delta \mathbf{y}^T \mathbf{W}_s \Delta \mathbf{y}}{r}, \quad (3.46)$$

with $\Delta \mathbf{y}$ the vector of residuals of the last iteration and r the degree of freedom. The iteration is stopped when the improvement of χ^2 compared to the last iteration is considered to be sufficiently small (e.g. $|\Delta \chi^2| < 10^{-6}$).

3.4.3. Lagrange Multipliers Algorithm

A second algorithm called *Lagrange Multipliers* was implemented for the calibration. Initial simulations showed that the sextupole transmission probabilities only converged in some rare cases with the Gauss-Newton method, this problem motivated the implementation of the Lagrange Multipliers algorithm. The algorithm is similar to the Gauss-Newton method and provides identical numerical results.

Only an outline of the derivation and the equations necessary for the implementation is shown in this section ⁴. The Lagrange multipliers algorithm treats the measured values the same way as the unknowns. The Taylor approximation of the function to be minimized includes Jacobian matrices for both the measurements and the unknown, whereas the Gauss-Newton algorithm only fits the model function to the data.

The r unknown parameters are combined in a r -vector $\mathbf{x}$. The real n measurable quantities are combined in a n -vector $\boldsymbol{\eta}$. The real values differ from the measurement $\mathbf{y}$ with an error ϵ : $\boldsymbol{\eta} = \mathbf{y} - \epsilon$. The errors $\epsilon_j (j = 1, 2, \dots, n)$ form the covariant matrix $\mathbf{C}_y$ (same as (3.15)) of the measured values $\mathbf{y}$. The weight matrix is defined as $\mathbf{W}_y = \mathbf{C}_y^{-1}$. The first estimate for $\mathbf{x}_0$ must be provided and the first approximation for $\boldsymbol{\eta}$ is $\boldsymbol{\eta}_0 = \mathbf{y}$. The values $\mathbf{x}$ and $\boldsymbol{\eta}$ are bound by the m functions

$$f_k(\mathbf{x}, \boldsymbol{\eta}) = f_k(\mathbf{x}, \mathbf{y} - \epsilon) = 0, \quad k = 1, 2, \dots, m. \quad (3.47)$$

The functions f_k are linearized with the following Taylor approximation:

$$\begin{aligned} f_k(\mathbf{x}, \boldsymbol{\eta}) &= f_k(\mathbf{x}_0, \boldsymbol{\eta}_0) \\ &+ \left(\frac{\partial f_k}{\partial x_1} \right)_{x_0, \eta_0} (x_1 - x_{10}) + \dots + \left(\frac{\partial f_k}{\partial x_r} \right)_{x_0, \eta_0} (x_r - x_{r0}) \\ &+ \left(\frac{\partial f_k}{\partial \eta_1} \right)_{x_0, \eta_0} (\eta_1 - \eta_{10}) + \dots + \left(\frac{\partial f_k}{\partial \eta_r} \right)_{x_0, \eta_0} (\eta_n - \eta_{n0}). \end{aligned} \quad (3.48)$$

⁴A detail of the algorithm can be found in chapter 9 and 10 in [96].

Using the abbreviations

$$a_{kl} = \left(\frac{\partial f_k}{\partial x_l} \right)_{x_0, \eta_0}, \quad \mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mr} \end{pmatrix}, \quad (3.49)$$

$$b_{kl} = \left(\frac{\partial f_k}{\partial \eta_l} \right)_{x_0, \eta_0}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{mn} \end{pmatrix}, \quad (3.50)$$

$$c_k = f_k(\mathbf{x}_0, \boldsymbol{\eta}_0), \quad \mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix} \quad (3.51)$$

and

$$\boldsymbol{\xi} = \mathbf{x} - \mathbf{x}_0, \quad \boldsymbol{\rho} = \boldsymbol{\eta} - \boldsymbol{\eta}_0, \quad (3.52)$$

Eq. (3.48) can be expressed as

$$\mathbf{A}\boldsymbol{\xi} + \mathbf{B}\boldsymbol{\rho} + \mathbf{c} = 0. \quad (3.53)$$

The solution to Eq. (3.53) is reached by improving the first approximations $\mathbf{x}_0$ and $\boldsymbol{\eta}_0$ in an iterative process:

$$\tilde{\mathbf{x}} = \mathbf{x}_0 + \tilde{\boldsymbol{\xi}} \quad (3.54)$$

$$\tilde{\boldsymbol{\eta}} = \boldsymbol{\eta}_0 + \tilde{\boldsymbol{\rho}}. \quad (3.55)$$

The improvements $\tilde{\boldsymbol{\xi}}$ and $\tilde{\boldsymbol{\rho}}$ for the unknown parameters $\mathbf{x}$ and measurements $\boldsymbol{\eta}$ are given by

$$\tilde{\boldsymbol{\xi}} = -(\mathbf{A}^T \mathbf{W}_B \mathbf{A})^{-1} \mathbf{A}^T \mathbf{W}_B \mathbf{c} \quad (3.56)$$

$$\tilde{\boldsymbol{\rho}} = \mathbf{C}_y \mathbf{B}^T \mathbf{W}_B (\mathbf{c} - \mathbf{A}(\mathbf{A}^T \mathbf{W}_B \mathbf{A})^{-1} \mathbf{A}^T \mathbf{W}_B \mathbf{c}) \quad (3.57)$$

with

$$\mathbf{W}_B = (\mathbf{B} \mathbf{C}_y \mathbf{B}^T)^{-1}. \quad (3.58)$$

The improved values (3.55) are used to recalculate the matrices in (3.53) for the next iteration.

The χ^2 is calculated after each iteration i :

$$\chi^2(i) = \frac{\mathbf{K}^T \mathbf{W}_y \mathbf{K}}{r}, \quad (3.59)$$

with $\mathbf{K}$ the vector of residuals and r the degree of freedom. After the final iteration the covariant matrix of the unknown parameters $\mathbf{x}$ and measurements $\boldsymbol{\eta}$ are given by

$$\mathbf{C}_{\tilde{\mathbf{x}}} = \mathbf{C}_{\tilde{\boldsymbol{\xi}}} = (\mathbf{A}^T \mathbf{W}_B \mathbf{A})^{-1} \quad (3.60)$$

$$\mathbf{C}_{\tilde{\boldsymbol{\eta}}} = \mathbf{C}_y - \mathbf{C}_y \mathbf{B}^T \mathbf{W}_B \mathbf{B} \mathbf{C}_y + \mathbf{C}_y \mathbf{B}^T \mathbf{W}_B \mathbf{A} (\mathbf{A}^T \mathbf{W}_B \mathbf{A})^{-1} \mathbf{A}^T \mathbf{W}_B \mathbf{B} \mathbf{C}_y. \quad (3.61)$$

The covariant matrix $\mathbf{C}_{\tilde{\boldsymbol{\xi}}} = \mathbf{C}_\epsilon$ together with the χ^2 value are used to calculate the systematic errors of the polarization as seen in Eq. (3.23).

3.4.4. LU Decomposition algorithm

A matrix inverse calculation is performed to calculate the polarization (3.8), to solve the iteration steps (3.42), (3.57) and also to extract the covariant matrices. The LU decomposition algorithm is an alternative method to the Gaussian elimination for determining an inverse matrix problem. Because the calibration calculations involve large matrices (≈ 3000) when fitting without average, the advantage of the LU decomposition is that it requires significantly less computing time for large matrices in contrast to the Gaussian elimination. The computing time for a $n \times n$ matrix inversion is proportional to [105]

$$T(n) \propto \frac{4n^3}{3} \text{ for the LU decomposition and}$$

$$T(n) \propto \frac{n^4}{3} + \frac{n^3}{2} \text{ for the Gauss elimination.}$$

The inverse matrix problem is used to solve the linear system $\mathbf{Ax} = \mathbf{b}$. If the matrix $\mathbf{A}$ is non singular, its inverse exists and the unique solution is $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$. If $\mathbf{A}$ possesses an inverse, the matrix can be factorized into two triangular matrices [96, 106]

$$\mathbf{A} = \mathbf{LU} \quad (3.62)$$

where $\mathbf{L}$ is a lower unit triangular matrix (has 1 on the diagonal and elements only below it) and $\mathbf{U}$ is an upper triangular matrix (with elements only on the diagonal and above). Using this decomposition, the linear system

$$\mathbf{A} \cdot \mathbf{x} = (\mathbf{L} \cdot \mathbf{U}) \cdot \mathbf{x} = \mathbf{L} \cdot (\mathbf{U} \cdot \mathbf{x}) = \mathbf{b} \quad (3.63)$$

is solved in two steps [107, 99]. With

$$\mathbf{L} \cdot \mathbf{y} = \mathbf{b}, \quad (3.64)$$

the solution for the vector $\mathbf{y}$ is used to solve $\mathbf{x}$ in

$$\mathbf{U} \cdot \mathbf{x} = \mathbf{y}. \quad (3.65)$$

The advantage of this approach is that the solution of a triangular set of equations is solved directly with forward or back substitution [108]. The corresponding system for the Eq. (3.64) is:

$$\begin{aligned} y_1 &= b_1 \\ L_{21}y_1 + y_2 &= b_2 \\ L_{31}y_1 + L_{32}y_2 + y_3 &= b_3 \\ &\vdots \\ L_{n1}y_1 + L_{n2}y_2 + L_{n3}y_3 + \dots + y_n &= b_n \end{aligned}$$

The first equation for y_1 can be solved directly. The solution is then substituted into the second equation to solve y_2 with

$$y_2 = b_2 - L_{21}y_1.$$

The value y_i is solved by substituting the values $y_1, y_2, \dots, y_{i-1}$ *forward* into the i th equation:

$$y_i = b_i - \sum_{j=1}^{i-1} L_{ij}y_j. \quad (3.66)$$

The *back substitution* used to solve (3.65) follows the same scheme by solving $x_n, x_{n-1}, \dots, x_1$ successively. The general solution is given by

$$x_i = \frac{1}{U_{ii}} \left(y_i - \sum_{j=i+1}^n U_{ij}x_j \right). \quad (3.67)$$

The LU decomposition to find the matrices $\mathbf{L}$ and $\mathbf{U}$ is performed using the Crout algorithm: the principle is to transform each matrix element A_{ij} of $\mathbf{A}$ into its final value L_{ij} for the lower matrix and U_{ij} for the upper matrix [107, 99, 109]. The procedure is as follows:

For each column $j = 1, 2, \dots, n$, the elements U_{ij} and L_{ij} are solved with

$$U_{ij} = A_{ij} - \sum_{k=1}^{i-1} L_{ik} U_{kj} \quad (3.68)$$

and then for each row $i = j + 1, j + 2, \dots, n$ the elements L_{ij} are given by

$$L_{ij} = \frac{1}{U_{jj}} \left(A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj} \right). \quad (3.69)$$

In (3.68) the summation term is zero when $i = 1$. Both procedures (3.68) and (3.69) are executed successively for each column j . Because every A_{ij} from the original matrix $\mathbf{A}$ is used only once, the values for U_{ij} and L_{ij} are stored *in place* into $\mathbf{A}$ which has the advantage to reduce the memory footprint. The decomposed matrix with elements m_{ij} contains the values for U_{ij} and L_{ij} . The diagonal elements U_{ii} are unity, but are not explicitly set in the matrix m . The $n \times n$ decomposed matrix has the following form:

$$\begin{pmatrix} U_{11} & U_{12} & \cdots & U_{1j-1} & U_{1j} \\ L_{21} & U_{22} & \cdots & U_{2j-1} & U_{2j} \\ \vdots & & & & \\ L_{i1} & L_{i2} & \cdots & L_{ij-1} & U_{ij} \end{pmatrix}. \quad (3.70)$$

The implemented algorithm uses the pivoting method to avoid numerical rounding problems. The principle is to interchange both the rows of the matrix $\mathbf{A}$ and the column of the vector $\mathbf{b}$ to place the largest number in the diagonal element U_{jj} in (3.69) during the decomposition [99]. In the final decomposed matrix the diagonal elements U_{ii} are still unity.

4. EXPERIMENTAL SETUP

4.1. Target Section Overview

The target section provides a polarized hydrogen or deuterium gas target for the PAX spin-filtering experiments. It is composed of the following main components: the Atomic Beam Source (ABS), the target chamber with the storage cell, the Target Gas Analyzer (TGA) and the Breit-Rabi Polarimeter (BRP). A schematic view of the components is shown in Fig. 4.1. High areal densities of up to 5×10^{13} atoms/cm² are required for spin-filtering. They are achieved by injecting nuclear spin polarized hydrogen or deuterium atoms produced by an ABS into a storage cell [110]. The BRP measures the polarization of an effusive beam extracted from that cell.

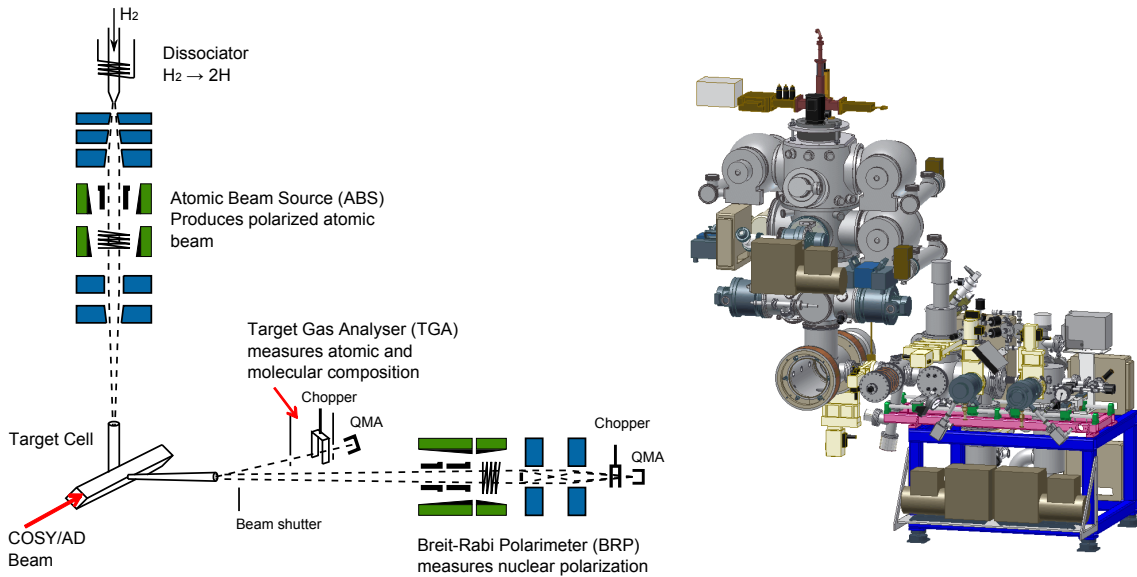


Fig. 4.1.: Schematic drawing (left-hand side) the Polarized Internal Target (PIT)[111] with the Atomic Beam Source (ABS, Sec. 4.2), the target cell (Sec. 4.3), the Breit-Rabi Polarimeter (BRP, Sec. 4.4) and the Target Gas Analyzer (TGA, Sec. 4.5). The right-hand side shows a 3D plot of the H-beam laboratory setup as used during the calibration measurements (source: technical drawing from IKP, Forschungszentrum Jülich).

4.2. Atomic Beam Source

The ABS, formerly used in the HERMES experiment [95, 112, 113], has been modified for the spin-filtering studies of the PAX experiment [111]. The vacuum system had to be modified because of space limitations of the future setup. The transitions in the appendix chamber of the ABS had to be removed because of the low target holding field requirement, and to increase the intensity by shortening the distance to the storage cell. The scheme of the ABS components is shown in Fig. 4.2.

For differential pumping the ABS is separated into 4 chambers (I-IV) and evacuated with 7 turbomolecular pumps. The pumping speed is approximately 10 000 l/s. This powerful pumping

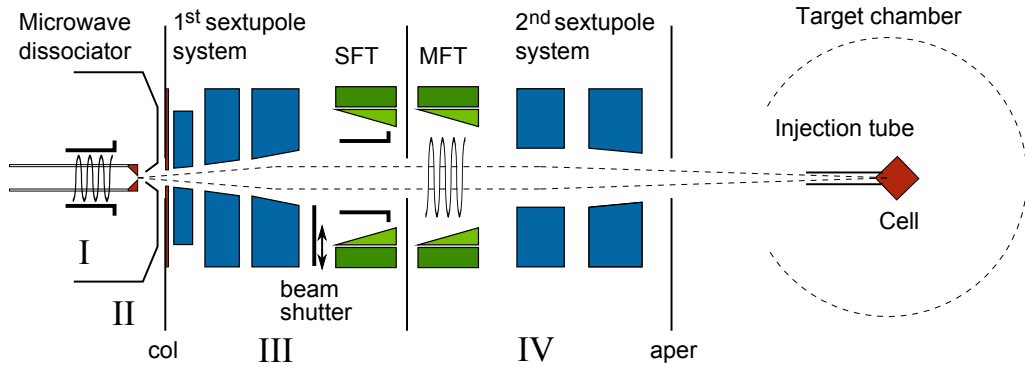


Fig. 4.2.: Schematic drawing of the ABS components installed in the chambers I to IV and the target chamber with the target cell. The ABS is separated from the test target chamber by a 20 mm aperture. (col: first collimator, SFT: strong-field transition unit, MFT: medium-field transition unit; aper: $\varnothing=20$ mm aperture).

system is necessary to limit the attenuation of the beam caused by residual gas produced during the beam formation and by the deflected hyperfine states (see below). The level of vacuum in the last ABS chamber (which contains the 2nd sextupole system) and of the test target chamber is in the order of 10^{-7} mbar*. The vacuum system is controlled by an independent PLC (Programmable Logic Controller) system[&], similar to the one developed for the ABS of ANKE at COSY [114].

The atoms (and a small fraction of undissociated molecules) leave the discharge tube towards the vacuum of the first chamber through a nozzle cooled to 100 K. In addition, to minimize the recombination of molecules, the main reason for the low nozzle temperature is to produce a cold supersonic beam in order to maximize the number of atoms into the velocity window of the sextupoles. The atoms then enter the second and third vacuum chamber by passing a skimmer and a collimator, respectively. The position of the nozzle relative to skimmer and collimator is optimized to match the supersonic beam to the acceptance angle of the first sextupole magnet [111, 115, 116]. Figure 4.3 shows a simplified scheme of the discharge tube, nozzle and skimmer.

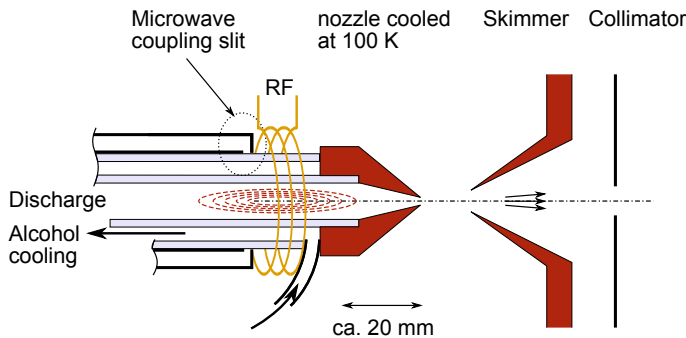


Fig. 4.3.: Schematic view of the dissociator and beam formation elements. A flow of 15°C alcohol cools the discharge glass tube. The nozzle is cooled at 100 K. The skimmer and collimator shape the atomic beam to match the acceptance of the first sextupole magnet [115].

The dissociator generates the hydrogen or deuterium atomic beam by dissociating molecules in a microwave induced low ionized plasma. The design is based on the waveguide surfatron dissociator [116, 117]. The 2.45 GHz microwave is produced by a magnetron powered by a DC power supply with a maximal nominal power of up to 1200 W. A circulator protects the magnetron from the reflected power [116]. Both the magnetron and the circulator are directly mounted on the waveguide surfatron. Because the discharge does not ignite with the microwave power alone, a radio frequency (rf) ignition coil is placed behind the microwave coupling slid. The coil is operated at 13.56 MHz and is powered up to 40-50 W until the microwave couples to the plasma. The rf coil should not be operated for longer than 20 seconds due to insufficient cooling.

The plasma is contained inside a glass tube with 1 to 2 mbar of hydrogen and 0.1 to 0.3 vol% of oxygen to improve the dissociation. The discharge tube is cooled to 15 °C by an alcohol flow inside

* In the final configuration the pressure in the target chamber will be much smaller.

[&]Siemens SIMATIC S7-300 controller and WinCC software.

the cooling tube. Water can not be used as a cooling agent as it would absorb the microwave. Typical hydrogen gas flows are in the order of 80-90 sccm[#]. The admixed oxygen reacts to H₂O and HO and leads to the creation of a water or ice layer which reduces the recombination mainly on the glass surface but also on the nozzle which is cooled to 100 K [116]. The ice build-up degrades the intensity over time by clogging the nozzle, which then needs to be evaporated after 3 to 5 days of operation. This procedure to remove the ice is called nozzle regeneration and takes about 3 hours to complete. The nozzle hole diameter influences the tube pressure and thus the velocity of the atoms. The maximum intensity of the injected beam inside the cell is reached when the beam velocity perfectly matches the sextupole optics and thus provides the best focusing power. The icing creates a bell shaped curve of the intensity over time (Fig. D.3 and 6.6). The oxygen admixture can be reduced when the tube is cooled to sub-zero temperatures; however, this requires an insulation of the cooling tube and of the flexible alcohol-feeding tubes to avoid water condensation and ice build-up.

The absolute ABS intensity is measured with a calibrated compression tube as explained in appendix D. During the BRP calibration and polarization measurements the injection intensity reached about 3.5×10^{16} atoms/s with the injection of states $|1\rangle + |2\rangle$. Further optimization will be carried on to reach the necessary intensity of 6×10^{16} atoms/s.

The purpose of the ABS is to inject a fully nuclear polarized atomic gas into the storage cell[118, 119] by injecting the hyperfine state $|1\rangle$ (Fig. 4.4). To perform this selection the ABS consists of a set of sextupole magnets, followed by two adiabatic rf-transition units and another two sextupole magnets (Fig. 4.2). The first sextupole system removes the states $|3\rangle$ and $|4\rangle$ and creates an almost fully electron polarized beam. In normal operation the MFT is set to the 2-3 transition to exchange the hyperfine state populations N_2 and N_3 . Because the population N_3 is almost zero after the first set of sextupole magnets, the MFT 2-3 transition effectively transpose all atoms of state $|2\rangle$ into atoms of state $|3\rangle$ which are then deflected to a high percentage by the second set of sextupole magnets. This combination of sextupole magnets and rf-transitions is arranged in the ideal case to transmit only the hyperfine state $|1\rangle$.

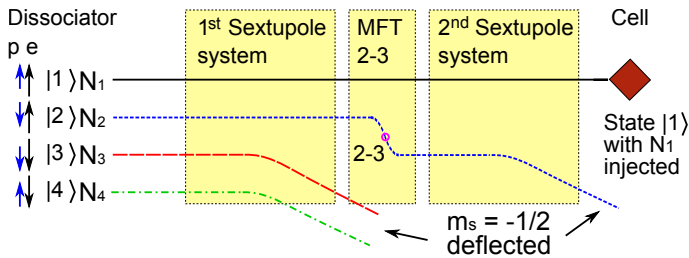


Fig. 4.4.: Schematic view of the ABS polarization injection for hydrogen. The sequence of sextupole magnets and rf-transition separates the hyperfine populations and selects in the ideal case only the state $|1\rangle$ for injection into the storage cell.

As seen in Sec. 2.3.1 only states $|1\rangle$ and $|3\rangle$ contribute to the polarization in a weak magnetic field. Therefore, only the injection of state $|1\rangle$ will be used during the PAX spin-filtering studies. All three injection modes, however, are used in the calibration procedure of the BRP. The mode MFT 1-2/2-3 is an alternative possibility to inject state $|1\rangle$ by selecting a negative gradient⁰. In this case the 1-2 transition operating prior to the 2-3 transition will not affect the occupation numbers. The injected states are therefore only affected by the efficiency ϵ_{m23} of the 2-3 transition. In the positive gradient configuration, the magnetic field settings must be selected in such a way that the 1-2 transition happening after the 2-3 transition is not active. Both positive and negative gradient configurations for state $|1\rangle$ reach the same efficiency. The possible hydrogen injection modes and operating parameters are shown in Table A.2. The ABS transitions are controlled with the same slow control system used for the BRP (Sec. 4.4 and 4.6).

[#] Standard Cubic Centimeters per Minute. 1 sccm = $\frac{1}{60 \cdot 1000}$ standard litre per second (slps).

⁰ A negative gradient has a decreasing field along the beam direction.

4.3. Target Chamber and Storage Cell

The target chamber hosts the storage cell and is connected to both the ABS and BRP. The test chamber described in this section was used to calibrate the BRP and to perform the first polarization tests; it will be replaced for the spin-filtering tests. The new chamber will contain the silicon detectors and the storage cell and will support the coils for the magnetic holding field. In addition, a new powerful pumping setup will pump the gas exiting from the cell. The test target chamber used during the calibration has a cylindrical shape with a diameter of 25 cm and a length of 58 cm. It is shown schematically in Fig. 4.5.

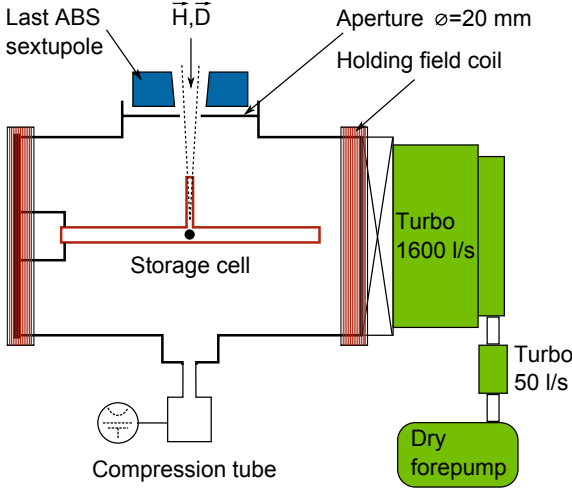


Fig. 4.5.: Schematic view of the target chamber hosting the storage cell. The compression tube is positioned below the cell on the ABS beam axis and is used to measure the absolute intensity of the beam from the ABS (in the open cell position). The storage cell is attached to a flange on one side of the chamber. A turbomolecular pump with a pumping speed of 1600 l/s is attached to the other side of the chamber.

Two coils are placed at both ends of the chamber to provide the magnetic holding field for the polarized gas. Two additional smaller coils are wound between the target chamber and the TGA (Fig. 4.12) along the extension tube to avoid any zero crossing of the magnetic field which occurs when the magnetic field reverses its direction. This effect induces depolarization effects which has to be avoided. The paired coils are each powered by a power supply controlled by the slow control software.

The purpose of the storage cell is to increase the dwelling time of the target gas atoms within the area of the beam, and thus to increase the target thickness. Compared with that of a jet target, an increase of two orders of magnitude is obtained. In a storage ring the lower thickness of a gas target compared to a solid target is compensated by the fact that the beam particles traverse the target at a frequency of about 10^6 s^{-1} . The main advantages of an internal polarized gas target are [120]: a high isotropical purity, the possibility of a fast spin reversal, low background due to the absence of container walls and no radiation damage because the gas is continuously replenished [92].

The luminosity necessary for spin-filtering requires a high areal density of up to $5 \cdot 10^{13} \text{ atoms/cm}^2$. This density can be achieved by minimizing the cell cross section. For a given intensity of the injected beam I_{in} , the areal gas density, n_{tg} (atoms/cm²), depends on the lengths l_{in} , l_{st} and the diameters d_{in} , d_{st} of the injection tube and the storage tube respectively [121]:

$$n_{tg} = \frac{I_{in} \cdot l_{st}}{2} \cdot \left[\text{const} \cdot \left(\frac{l_{in}}{d_{in}^3} + \frac{l_{st}}{d_{st}^3} \right) \right]. \quad (4.1)$$

To achieve an areal density as high as possible, the lengths have to be as large as possible and the diameters as small as possible. The dimensions of the feeding tube are limited by the divergence of the incoming beam from the ABS and l_{st} is limited by the available space. Thus, d_{st} or the lateral dimensions for a non-circular tube cross section have to be made as small as possible during the measurements. This requirement can be reached with a cell which is widened during injection of the beam into the storage ring and closed after beam manipulation (injection and phase space

cooling). The Antiproton Decelerator (AD) storage ring at CERN requires a 100 mm aperture at the injection energy of 3.57 GeV. After cooling and ramping down to 40-450 MeV the quadrupole magnets are able to focus the beam to a cross section of 10 mm. The cell construction, shown in Fig. 4.6, corresponds to these boundary conditions. During injection and ramping down the beam from the ABS is blocked and the two halves of the cell are separated (Sec. 6.2.2 analyzes the polarization stability related to the cell movement). When the required energy is reached the cell is closed and the ABS beam is switched on. The cell to be used has a length of 400 mm and a square cross section of $10 \times 10 \text{ mm}^2$. The injection tube and the BRP sampling tube are placed at the center. The cell walls are made from a $5 \mu\text{m}$ Teflon foil which is known to reduce depolarization and recombination [122]. Additionally, the thin foil allows low-energy particles to pass through and reach the detectors.

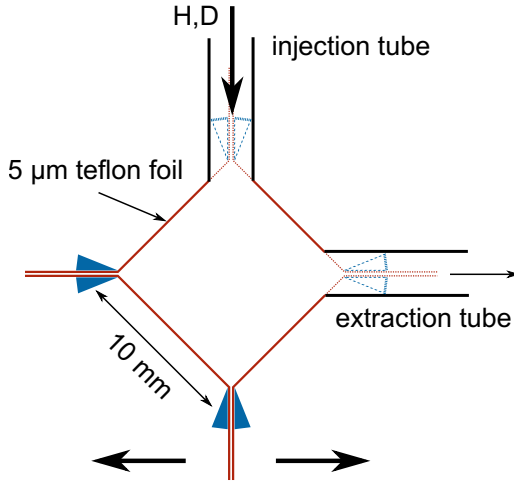


Fig. 4.6.: Cut through the center of the storage cell. The cell is composed of four assembled quarters. For each quarter the Teflon foil is clamped between two rods machined from aluminum. The polarized atomic beam is focused by the last sextupole magnet and is injected from the top. The sampling tube enables atoms to leave the cell into the BRP which measures the polarization of that sample. The left-hand and right-hand halves of the cell are moved to open the cell.

The operation at the COSY ring will not require the cell opening because the beam is injected at low energy and can be squeezed through the cell by the quadrupole magnets even when it is still uncooled. A prototype of an openable storage cell was used during this work. Photographs of the cell inside the target chamber in position closed and open are shown in Fig. 4.7.

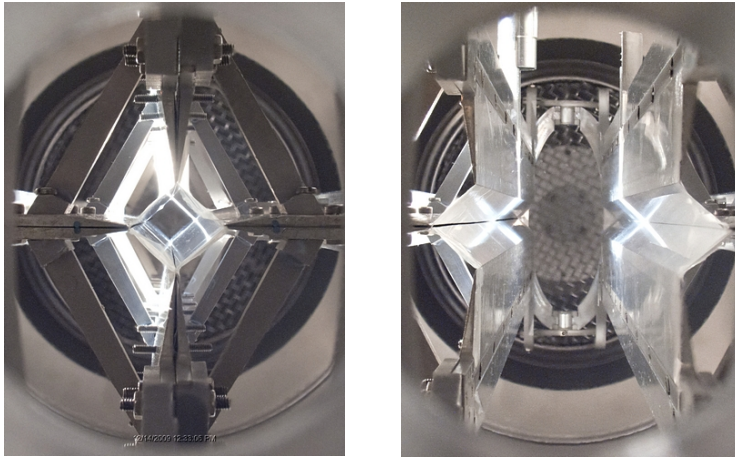


Fig. 4.7.: Photograph of the storage cell installed in the target chamber in the positions “closed” (left-hand side) and “open” (right-hand side). The injection tube moves with the left half of the cell and can be seen in the right photograph on the top left half of the cell.

4.4. Breit-Rabi Polarimeter

The components of the Breit-Rabi polarimeter are the rf transition units, the sextupole system and a Quadrupole Mass Analyzer (QMA) measuring the beam intensity (Fig. 4.8). It is mounted on two rails to allow decoupling the polarimeter from the target chamber. A window at the end of the BRP is used to align the QMA optics with the beam blocker and the cell.

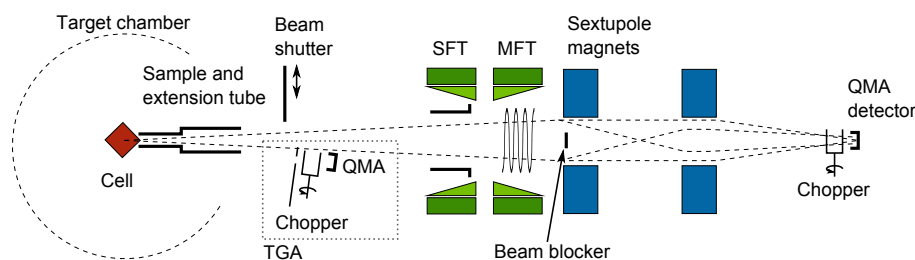


Fig. 4.8.: Schematic front view of the BRP components. The BRP itself is composed of two adiabatic high-frequency transitions followed by two sextupole magnets. A QMA with chopper measures the beam intensity.

4.4.1. Vacuum System

The Breit-Rabi Polarimeter, developed for the HERMES experiment [85], has to measure beam intensities of the order of 10^{-11} mbar-l/s. Sensitivity to such a low intensity beam requires ultra high vacuum conditions, especially in the detector chamber. Molecules containing hydrogen such as water or H_2 will produce hydrogen ions in the ionization volume of the QMA and they contribute to the background signal.

Three vacuum chambers, designed to enable the ultra high vacuum, host the BRP components. Two of them are installed in a common vacuum vessel as shown in Fig. 4.9. The first chamber hosts the TGA, the second chamber contains the high-frequency transition units and the sextupole magnets, and the detector chamber contains the BRP QMA detector. This chamber is connected to the sextupole chamber by a 200 mm long and 35 mm diameter bellows and an electro-pneumatic DN35 valve. The small diameter limits the conductance between both chambers to reduce the background. The detector chamber is mounted on an adjustable structure for alignment.

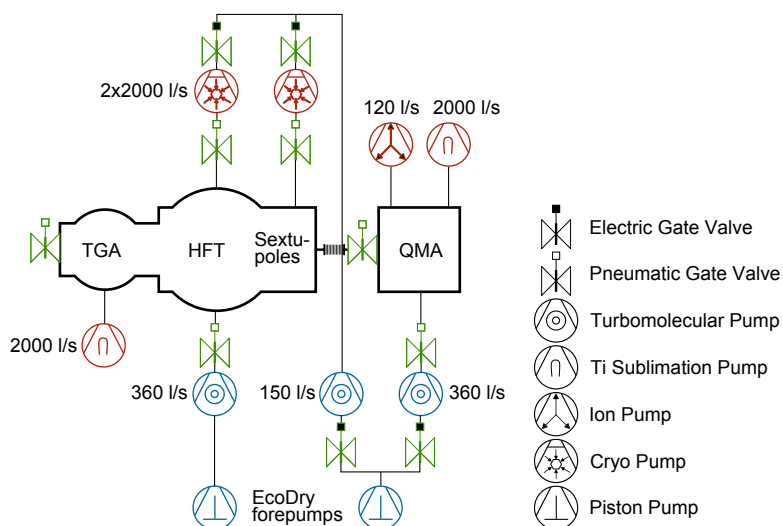


Fig. 4.9.: Schematic view of the BRP pumping system. The TGA chamber and the chamber with the HFT and sextupole magnets share the same volume.

The TGA chamber is pumped by a 2000 l/s titanium sublimation pump and is separated from the target chamber by a DN100 CF valve. The HFT and sextupole chamber is pumped by two 2000 l/s cryopumps to remove the defocused hyperfine states of hydrogen or deuterium (cryopumps have a high pumping efficiency for those gases). This chamber is initially evacuated by a 360 l/s turbomolecular pump. An additional 150 l/s turbomolecular pump is used to regenerate the cryopumps in a separate volume. The detector chamber is evacuated by a 360 l/s turbomolecular pump. To reduce the residual gas background a titanium sublimation pump of 2000 l/s pumping speed for hydrogen and deuterium is located directly below the detector. The pump is typically operated with a 40 A sublimation period of two hours. Heavier gases are pumped by a 120 l/s ion getter pump. The cryopumps and all turbomolecular pumps can be separated from the

chambers with electro-pneumatic gate valves. The turbomolecular pumps are connected to two dry compressing piston forepumps.

To fulfill the ultra high vacuum conditions the TGA and BRP chambers are heated for 24 to 48 hours to 150-200 °C in a bake-out procedure. The heating accelerates the outgassing of impurities and water adsorbed by the chamber walls [123]. Thermocouples connected to Proportional-Integral-Derivative (PID) controllers assure that sensitive components like feed-through, vacuum gauges and the QMA do not exceed the permitted temperature. The sextupoles magnets are water-cooled during the bake-out process to keep their temperature well below the Curie temperature and thus to avoid demagnetization.

4.4.2. High-Frequency Transitions

To change the population of hydrogen or deuterium hyperfine states two adiabatic high-frequency transitions are used in the BRP: a Strong Field Transition (SFT) unit and a Medium Field Transition (MFT) unit. The transitions are operated at fixed frequencies and the transition condition is reached by selecting the optimal gradient and homogeneous magnetic fields (Sec. 2.4.3). Both superimposed magnetic fields are perpendicular to the atomic beam.

Medium Field Transition

The MFT unit (Fig. 4.10) is operated below 100 MHz and uses a coil to generate the rf field. The variable frequency makes it possible to operate the unit with hydrogen and deuterium. The rf field is perpendicular to the static homogeneous and gradient magnetic fields. An rf oscillator unit is connected to an amplifier and feeds the coil with an adjustable frequency. The operation in a medium field ($B \approx 0.1B_C$) combined with a gradient field allows one to separate the transitions 1-2 and 2-3 (and 3-4 for deuterium). By varying the homogeneous component of the field, it is possible to run either the transition 1-2 and 2-3 successively or separately 1-2 or 2-3 [124, 125].

A Collins filter connected between the amplifier and the coil enables to match the system impedance to 50 Ω . The Collins filter consists of a moving coil and two grounded variable capacitors. A one loop coil installed close to the main coil acts as pick-up coil; it is connected to an oscilloscope to measure the pick-up amplitude. The elements of the Collins filter are tuned to maximize this amplitude. The main coil can be tuned within a 40 MHz band; however, not all modes will provide enough amplitude to operate the transition at a high efficiency. The frequency with the highest pick-up amplitude was selected for the BRP calibration.

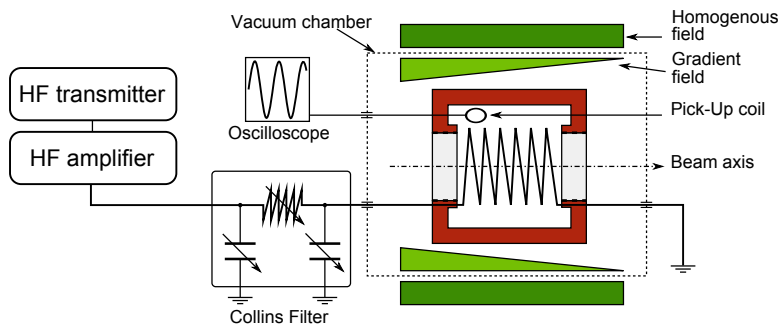


Fig. 4.10.: Schematic view of a MFT high-frequency transition unit [85]. The pick-up signal is displayed with an oscilloscope to tune the frequency, amplitude and filter.

Strong Field Transition

The SFT unit (Fig. 4.11) requires an rf field with a frequency higher than the respective hyperfine structure energy separation at zero field, i.e., $\nu_{SFT} > 1420$ Mhz for hydrogen and $\nu_{SFT} > 327$ MHz for

deuterium. This rf is generated by a band-conductivity resonator [85, 126]. The resonator is a copper cavity with two tilted copper rods. In one of the rods an oscillation is excited by a coupled high-frequency. The rf field emitted by the excited rod couples to the second rod and excites an oscillation there too. The emitted waves from the two rods together with wall reflections superimpose to a standing wave with two main modes. The oscillations in the two rods can be either in a parallel or anti-parallel phase. In the latter case the high-frequency magnetic field will constructively interfere between the two rods at the beam axis. This mode is used for the strong field transition.

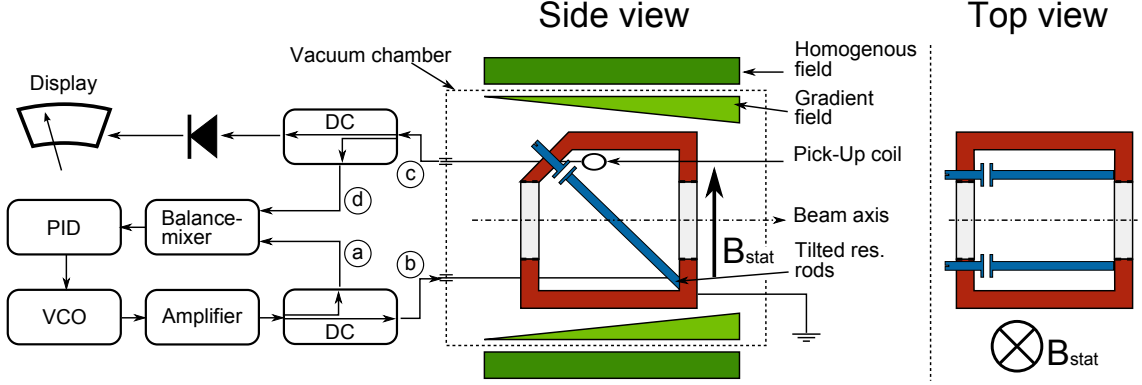


Fig. 4.11.: High-frequency SFT unit. The cavity resonance condition is kept by controlling the supplied frequency with a feedback loop. It uses a balance mixer and a voltage-controlled oscillator. The cable lengths have to fulfill the condition $b - a = c + d$ [85]. The resonator rods are tilted relative to the beam axis and to the static magnetic field to enable σ and π transitions.

Ideally the resonator rods have a length of $\lambda/4 \simeq 5.25$ cm ($\lambda/4 \simeq 22.8$ cm for deuterium) with one grounded and one open end. A current minimum (and voltage maximum) is induced at the open end with the oscillating field. The effective rod lengths can be reduced by capacitive loads at the open ends (ch. L 9 in [127]). Variable capacitors make it possible to change the resonance frequency. A shorter construction than imposed by the $\lambda/4$ constraints reduces the distance to the first sextupole magnet and shortens the distance from the storage cell to the QMA. A compact construction of the polarimeter is desirable to increase the acceptance angle of the QMA detector and thus the signal intensity.

To enable both σ and π transitions the magnetic field has to oscillate with a component parallel and perpendicular to the static magnetic field, as discussed in Sec. 2.4. Therefore, the resonator rods are tilted relative to the static field as shown in the side view of Fig. 4.11. A new layout for the SFT cavity has the rods tilted relative to the static magnetic field, but parallel to the atomic beam. This geometrically simplified construction will make it possible to accommodate two pairs of rods within the same cavity for both hydrogen and deuterium frequencies. In the actual setup both gases require two dedicated cavities which have to be exchanged.

The high-frequency power fed into the cavity (P_{HF} in the order of Watts) heats the rods and therefore modifies the capacity. The resulting frequency shift is corrected by the feedback loop using a Balance Mixer [85] and a PID controller. The supplied power and the pick-up signal are compared in a Balance Mixer using directional couplers (DC). In the resonance case the phase difference in the Balance Mixer between the coupling and pick-up signal is $\pi/2$. This condition is reached when the cable length between the Balance Mixer, the DCs and the cavity fulfill the condition $b - a = c + d$ [85] as illustrated in Fig. 4.11. A PID controller uses the input signal of the Balance Mixer and adjusts the emitted frequency using a voltage-controlled oscillator (VCO) to keep the cavity in resonance. The signal of the pick-up coil is cut by a diode and displayed by a voltmeter and can also be used to tune the frequency to the cavity resonance.

The frequency shift created by the controller has consequences for the tuning because the transition resonance is based on a fixed frequency. This is usually not a problem since the resonance curve

has a plateau as the transition conditions are kept by the shift along the gradient magnetic field. The SFT 1-4 transition resonance, however, has no plateau and a frequency shift could influence the transition efficiency. Furthermore, the PID controller does not support the remote suppression of the amplitude and will not resume operation when the transition is switched off and on again. Therefore, when using the controlled frequency, the transition has to be switched by the amplifier and not by the controller.

The controlled or uncontrolled frequency modes are both a compromise. An uncontrolled frequency could shift outside of the resonance and reduce the field amplitude necessary for the transition and thus change the efficiency. A controlled frequency mode, however, while guarantying maximal amplitude, shifts the transition frequency which can also reduce the efficiency. An uncontrolled frequency operation is possible when the cavity has reached a stable operating temperature. The calibration and polarization measurements in this work did not use the controlled frequency mode.

4.4.3. Sextupole System

The BRP was previously used in the HERMES experiment [128, 129] with a sampling of the target gas thermalized from the cell cooled at 100 K. The actual configuration for the PAX spin-filtering studies make use of a storage cell at room temperature. This requires a new magnet configuration since the atoms extracted from the storage cell move faster. The new sextupole magnet configuration uses a single magnet for the first section and two combined magnets for the second section [130, 91] (Table 4.1).

Table 4.1.: Sextupole magnets configuration.

Distance from cell center /mm	length /mm	bore /mm	pole tip field /T	aperture radius /mm
850	99	23	1.47(4)	12.9 ± 0.3
1150	99+72	23	1.47(4)	12.9 ± 0.3

A circular beam blocker placed in front of the first sextupole magnet blocks atoms with a trajectory close to the axis where the separating force is weak (see Sec. 2.5). This ensures that atoms with negative electron spin (states $|3\rangle$ and $|4\rangle$) which are deflected by the Stern-Gerlach force will not reach the QMA. The presence of the beam blocker permits to set the transmission probabilities σ_3 and σ_4 to zero and to only consider the unknowns σ_1 and σ_2 . Furthermore, because the detector measures always the sum of the the final states σ_1 and σ_2 . With the normalization $I_{tot} = \sum_a I_a$ and $n_a = I_a/I_{tot}$ (see Sec. 3.2), only the ratio σ_2/σ_1 must be calculated during the calibration [71, 131].

4.5. Target Gas Analyzer

The Target Gas Analyzer (TGA) is used to measures the relative amount of atoms and molecules coming from the cell. The recombination reduces the polarization in the cell¹ and thus needs to be taken into account [133, 134]. The TGA is located between the storage cell and the BRP HFT units. Its vacuum chamber shares the same volume as the transition units and the sextupole system. The intensities are measured by a quadrupole mass analyzer (QMA). A chopper is used to subtract the background. Two apertures, one placed just in front of the chopper and the second in front of the ionization volume of the QMA, ensure that only atoms or molecules from the extension tube can

¹The nuclear polarization of the molecules also depends on the cell surface and holding magnetic field [132].

reach the detector. Additionally, the apertures ensure that the atoms do not recombine on the wall of the ionization volume as this would increase and falsify the recombination ratio. The apertures, the chopper and the QMA are placed at an angle of 7° off axis to not interfere with the atomic beam for the BRP (Fig. 4.12). The TGA uses the same data acquisition method and signal processing as the BRP (see Sec. 4.6).

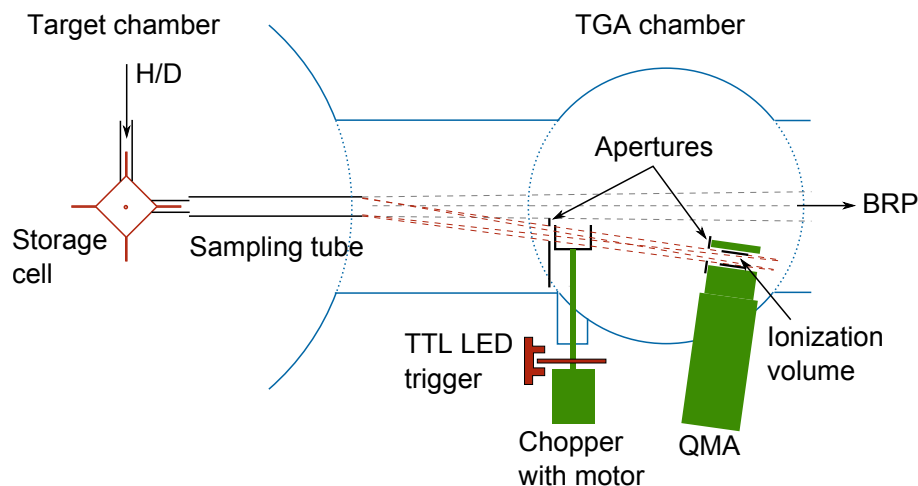


Fig. 4.12.: The Target Gas Analyzer (TGA) with the beam chopper and the Quadrupole Mass Analyzer (QMA) located at a 7° angle relative to the effusive beam axis [71]. The TGA is used to determine the relative amount of atoms and recombined molecules effusing from the cell. The chopper motor also drives a wheel with two slits to generate a trigger with a TTL LED.

4.6. Detection System and Data Acquisition

Both the TGA and BRP use the same beam detection method consisting of a chopper with trigger, a quadrupole mass spectrometer and a data acquisition system. The chopper is located in front of the ionization volume and periodically interrupts the beam to enable the background subtraction.

4.6.1. Quadrupole Mass Analyzer

The detector used to measure the beam intensity is a QMA (Balzers QMA400 [135]) which consists of a crossbeam ion source, a quadrupole mass filter and a channel electron multiplier (CEM or channeltron) (Fig. 4.13).

Atoms or molecules entering the ionization volume are ionized by 70 eV electrons emitted by a heated filament. The ions are extracted from the ion source and focused into the quadrupole mass filter. The alternating electric field of the quadrupole rods let only a specific mass to charge ratio of the particles pass through the filter. After that the ions are deflected into the channeltron and release one or more secondary electrons. The electrons are accelerated to 2 keV and trigger an electron avalanche which generates a charge pulse in the CEM anode.

The rotating field of the quadrupole rods is controlled by the QMA 400 rf generator which is controlled by a custom made NIM module. The resolution and mass selection are controlled by the LabView program while the ion optic voltages are set manually (Fig. E.1). Additionally, the overall mass range and sensitivity of the rf generator can be changed manually in order to optimize the signal for a specific mass range. Those settings influence the linear dependence between the mass and the control voltage and also change the shape of the signal. The two QMAs are optimized for the mass range of 0-90 amu. Once tuned, the rf settings and ion optics should not be changed

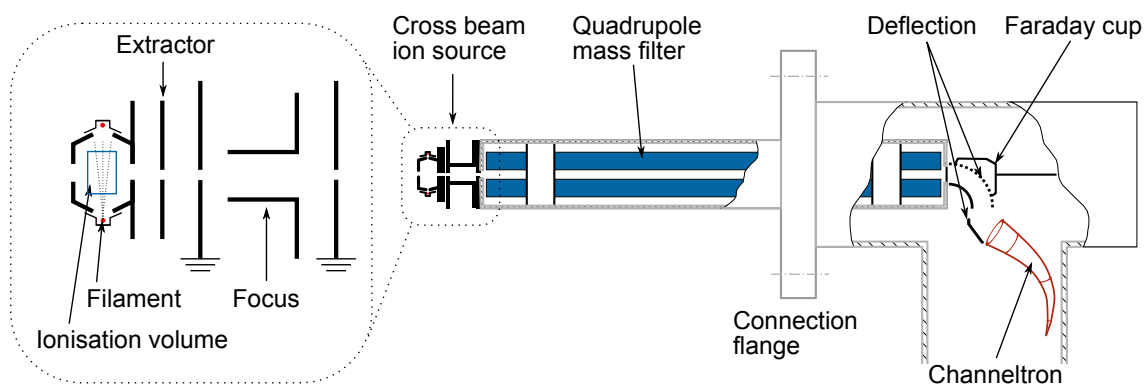


Fig. 4.13.: Schematic view of the quadrupole mass analyzer [135]. The left side shows the details of the ionisator (see also appendix E). Atoms or molecules are ionized in the cross beam ion source volume, accelerated by a high voltage and focused into the quadrupole mass filter. By using an rf field only one mass to charge ratio has a stable trajectory through the filter and exits at the deflection point. The ions are detected by secondary electron avalanche in the channeltron.

anymore. The optimal operating voltage of the channeltron changes over time and needs to be determined with a channeltron scan. Also the control voltage dependence on the atomic mass must be calibrated for each QMA. (See appendix E for more details and used parameters.)

4.6.2. Data Acquisition

The data acquisition system records two types of signals. The first system acquires the QMA pulses with a fast counter and the second system records analog voltages with an Analog to Digital Converter (ADC). The data acquisition and slow control software is programmed with the software package LabView (National Instruments [136]) running on a standard personal computer with Windows XPTM.

The QMA pulses are amplified by a fast amplifier placed at a close distance of about 1 meter from the QMAs to minimize signal attenuation and external interferences. The amplified pulses are converted into NIM pulses with a discriminator. The NIM pulses are sent to a shielded connector block (model SCB-68) which is connected to a 32-Bit counter card (model NI PCI-6602). The counter card located inside the computer is connected to the standard PCI 32-bit bus and is controlled by the LabView software. This setup enables single ion counting for both QMAs (TGA and BRP) of up to one MHz.

The analog signals recorded during the BRP operation are typically slow changing voltages from various devices like pressure gauge, power supply monitor and filament emission current. The voltages are acquired by a CAMAC ADC and read by a GPIB²-to-CAMAC interface (model LC 8901A.). The GPIB interface can listen and talk to any CAMAC modules and appears as a single instrument in the LabView programming concept. The GPIB board is connected via USB to the computer. The data acquisition setup is shown schematically in Fig. 4.14.

4.6.3. Signal Processing

The BRP and TGA intensity measurements are based on atomic and molecular flow passing through the QMA ionization volumes. Such low flow rates in the order of 10^{-11} mbar·l/s [85] require a single

²General Purpose Interface Bus (GPIB).

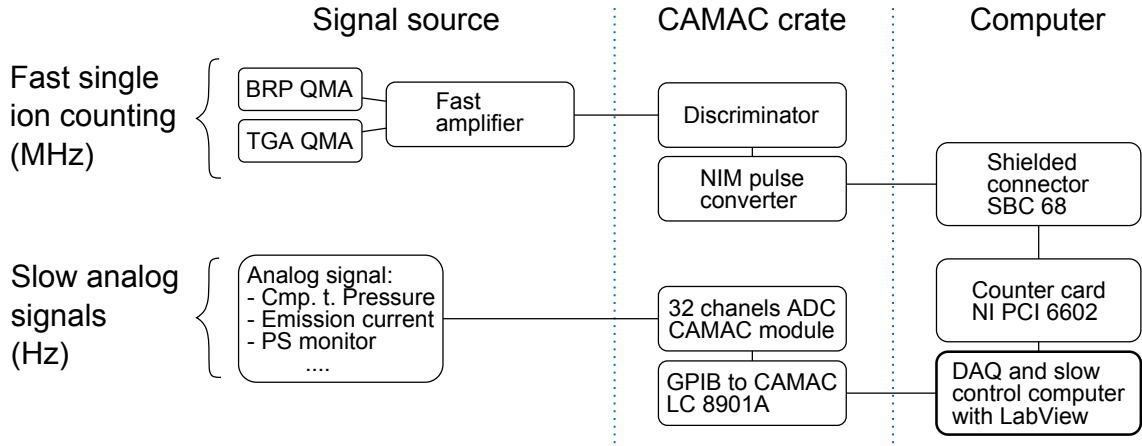


Fig. 4.14.: Schematic view of data acquisition setup. The acquisition is separated into two independent paths: fast QMA pulses are counted by a counter card, and analog signals are acquired with a CAMAC ADC module using a GPIB interface connected with USB.

ion counting technique with a channeltron to be able to subtract the background induced by the residual gas.

A fork shaped chopper placed in front of the QMA periodically interrupts the incoming beam and rotates at a frequency of 2.5 to 3 Hz. The chopper trigger generated by a LED is in phase with the rotating fork and is used to set the time boundaries for one rotation. Both the trigger and the QMA pulses are recorded by the counter card and the counted pulses are integrated in a time histogram. The correlation of the chopper position, trigger signal and counts is illustrated in Fig. 4.15. Each counted ion is accumulated into a given time interval bin of the histogram. The number of bins per cycle is typically set to 100 or 500 and the bin length is adapted to the chopper frequency. The chopper is driven by a DC motor with a frequency variation of up to 2%, the frequency is therefore measured in parallel and used to continuously adapt the histogram sampling frequency. The count rate is normalized to 1 s^{-1} .

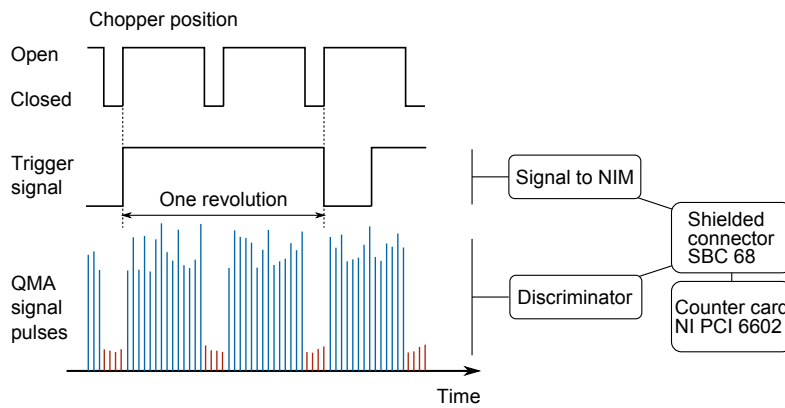


Fig. 4.15.: Illustration of the signal processing. The chopper triggers once per revolution. The trigger and ion counts are recorded by the same counter card and are synchronized in the software.

The time spectrum histogram is averaged for typically 5 to 30 cycles depending on the required statistical error. The signal is the difference between the closed position which measures the background and the open position which measures the sum of signal and background. The signal error is directly extracted from the observed variation for the count rates. Because the background is correlated to the signal, the errors are added linearly. Supposing n bins with x_i counts are acquired in the open position (signal+background) and m bins with x_j counts are acquired in the closed position (background), the standard error of the signal is calculated with

$$\delta S = \frac{1}{n-1} \sum_{i=1}^n (x_i - \mu_i) + \frac{1}{m-1} \sum_{j=1}^m (x_j - \mu_j), \quad (4.2)$$

where $\mu_{i,j}$ are the count average in the open and closed chopper position respectively.

An example of a time histogram with 500 bins averaged over 1000 cycles is shown in Fig. 4.16. The signal is the difference between the open and closed position. The chopper position boundaries can be changed in the online and offline software analysis.

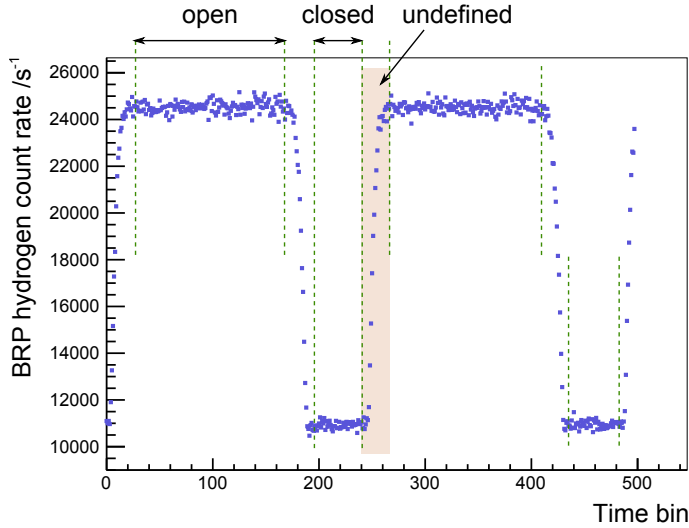


Fig. 4.16.: QMA signal vs. time spectrum histogram for one revolution averaged with 1000 cycles. The vertical dashed lines show the chopper position boundaries. The counts inside the undefined area between the open and closed positions are ignored.

4.6.4. Data Analysis

Each raw time spectrum requires additional acquisition parameters for the analysis, like the binning parameters and also information about correction factors, like the emission current. Therefore, each time spectrum measurement must be accompanied by the machine parameters used for the transition and also slow changing values such as the QMA emission current.

The polarization and the calibration acquisition process consists of multiple measurements with different transition modes in order to reach an overdetermined system as discussed in Sec. 3.2. In both cases the measurements follow the same procedures, the difference being that a calibration routine uses multiple ABS injection modes and also all BRP modes are used while the polarization measurement uses only one defined ABS setting and does not require all BRP modes. The raw data acquisition and file structure is therefore identical for both polarization and calibration measurements.

The data files have the following structure. For each measurement of a mode the relevant machine parameters as well as the required analog signals are combined into a header followed by the raw time spectrum of the count rate. These combined data represent a single mode acquisition. All polarization (or calibration) modes are measured sequentially and stored in a single file. This file includes all necessary information for the offline analysis and covers one full day of operation. A calibration data file includes only the calibration modes acquired during the calibration routine which lasts from 2 to 3 hours. The online polarization analysis is based on the last 4 to 11 modes only. The data file creation for the data analysis is illustrated in Fig. 4.17.

4.7. Slow Control System

The slow control system consists of a computer running LabView, a GPIB-to-CAMAC interface and 5 digital to analog converters (DAC) boards. The LabView software controls the CAMAC DAC via the GPIB interface using a USB connection. The 5 CAMAC DAC modules have each 8 channels with an output voltage of 0 ± 10 V with a 12 bit resolution. The controlled target components are

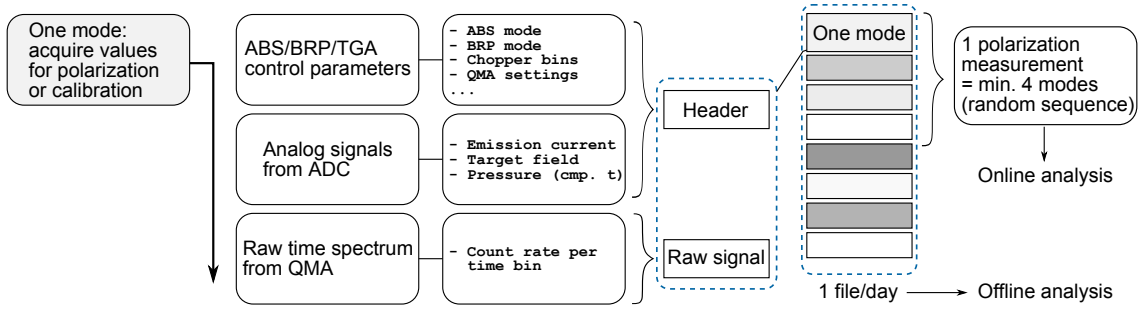


Fig. 4.17.: Schematic illustration of the data analysis. Each measurement mode is a combination of a header including the machine status and analog values and the raw time spectrum in form of count rates per time bin. The online polarization analysis for hydrogen is based on the last 4 to 11 measured modes. All measured modes are stored sequentially into a single file once per day which is used for the offline analysis.

the high-frequency transitions, the QMAs, the holding field coils and the beam shutter. The control chain from the computer to the hardware for one transition measurement is illustrated in Fig. 4.18.

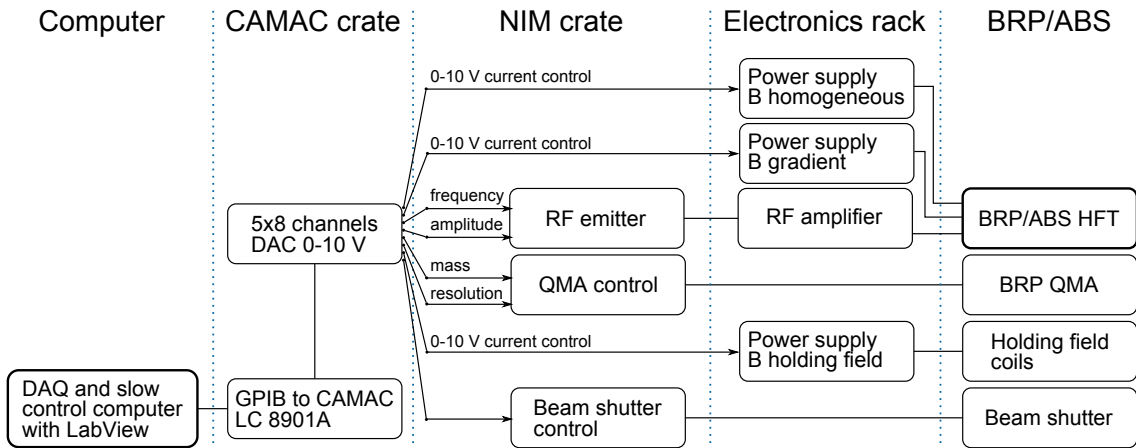


Fig. 4.18.: Schematic illustration of the slow control system. Control components active for the measurement of a single high-frequency transition plus beam shutter and holding field.

The QMAs are controlled with two voltages from the LabView software. The first voltage is the resolution value and influences the width of the mass peaks. The second voltage controls the mass selected by the quadrupole filter. The voltages are supplied to a custom made NIM module which bundles the QMA optic voltages and controls the rf generator with the provided resolution and mass values. For a mass scan, used to analyze the vacuum rest gas or fine tune the mass position, the mass voltage is ramped from 0 to 10 volts while acquiring the QMA count rate. The 0-10 volt range covers a mass range of $\approx 0-90$ amu. An example of a mass spectrum is shown in Fig. E.3. During a normal polarization or calibration operation, the mass is set to 1 for hydrogen or 2 for deuterium in the BRP.

The high-frequency transitions require the control of the high-frequency rf field and the static magnetic fields. The time-dependent magnetic field (rf) is controlled by the frequency and amplitude of the emitter with a 0-10 V input voltage for each value. The static magnetic fields are created by homogeneous and gradient magnetic field coils each controlled by a power supply. The power supplies are controlled by a 0-10 V input voltage which covers the full power supply output range. The used power supplies for each transition coil are listed in Table A.1 together with their connection to the DAC.

5. CALIBRATION OF THE BREIT-RABI POLARIMETER

5.1. Calibration Parameters

5.1.1. Signal Modes and Calibration Variables

Each BRP and ABS mode is labeled using the name and order of the active transitions; for example, the signal resulting only from the active SFT 1-4 transition is called s14. The MFT has multiple sub-transitions which are arranged according to the gradient direction. In the BRP the MFT gradient is negative because, as discussed in Sec. 2.4.3, Eq. (2.79), with a positive gradient the double transition m23m12 is identical to the m23 transition with respect to the signal intensity behind the sextupole magnet. On the other hand, the ABS MFT can in principle use both gradients to inject the state $|1\rangle$. The BRP MFT modes for hydrogen are m13 and m23, while m13 indicates that first the MFT 1-2 and then MFT 2-3 are active. The ABS positive gradient provides the modes m23m12 and m23 (in this case the transition 1-2 is not active), and the negative gradient can produce the mode m12m23.

The close proximity of the high-frequency transition (HFT) units in the BRP, necessary to reduce the distance to the QMA, induces a so-called magnetic field cross talk between the two HFTs. This means that different magnetic field settings on one transition will also influence the field strength on the other transition. The disturbance, however, differs between the SFT and MFT because the difference of the magnetic field strength between the SFT 1-4 and SFT 2-4 ($\Delta B \approx 8$ mT) is about ten times larger than between the MFT 1-2 and MFT 2-3 ($\Delta B \approx 0.6$ mT) (see also Fig. 2.5).

Due to the smaller magnetic field separation of the MFT sub-transitions, the SFT transition efficiencies are not affected by the MFT setting. In contrast to that the cross talk of different SFT settings is larger and leads to a situation where the MFT transition is out of resonance. Therefore, the MFT modes are defined together with an SFT magnetic field value and their number is increased by the number of SFT transitions (2 for hydrogen and 4 for deuterium). The magnetic field setting of the SFT used together with an MFT transition is denoted by the letter c (for calibration). For example, the MFT 1-3 transition exists as m13c14 and m13c24 respectively for the SFT 1-4 and 2-4 magnetic field settings without SFT rf on. The letter s denotes the active mode of the SFT (e.g., m13s24).

All possible BRP signal modes are composed of the SFT and MFT modes including combinations of both and also the r_{off} setting. This “off” setting, with the rf of both transitions switched off, will allow the states $|1\rangle$ and $|2\rangle$ to pass through the sextupole magnets and reach the BRP QMA. The states $|3\rangle$ and $|4\rangle$ are removed from the beam. The magnetic fields are kept active in the r_{off} mode to avoid any zero-crossing (see Sec. 4.3). The 11 possible BRP signal modes for hydrogen are shown in Table 5.1.

The transition efficiencies are denoted with the subscript ϵ and are followed by the transition name like ϵ_{s14} or ϵ_{m13} . As seen in Sec. 3.2 all MFT sub-transitions must be taken into account even when a sub-transition is not supposed to occur. The MFT multiple sub-transitions are denoted by the letter r . For example, the MFT 2-3 transition is characterized by the two sub-transitions ϵ_{m23r23} and ϵ_{m23r12} denoting the sub-transitions 2-3 and 1-2. Ideally the sub-transition ϵ_{m23r12} is equal zero. As seen for the signal modes, due to the magnetic cross talk, each MFT efficiency is related to a specific

SFT setting which is denoted by the letter c . Including cross talk the total number of transition efficiencies is 10 for hydrogen. Without cross talk the number of efficiencies would be 6 (2 SFT and 4 MFT).

The beam blocker in front of the sextupole magnets fully rejects the states $|3\rangle$ and $|4\rangle$ (see Sec. 4.4.3) and reduces the transmission probabilities of the sextupole magnets to the single unknown ratio σ_2/σ_1 . Thus, for hydrogen the total number of calibration unknowns is 11. All hydrogen calibration variables and their transition settings are listed in Table 5.2. The signal modes and calibration variables for deuterium use the same nomenclature and are listed in appendix B.

Table 5.1.: BRP signals for hydrogen. The two MFT modes 2-3 and 1-3 are measured twice with different SFT magnetic field settings. The magnetic fields of the transitions are active for the OFF mode to avoid a zero-crossing, in this case only the rf emitters are switched off.

BRP mode	signal name	SFT-RF	SFT-B	MFT-RF	MFT-B
RF-OFF	rfoff	OFF	ON	OFF	ON
SFT 1-4	s14	ON	1-4	OFF	ON
SFT 2-4	s24	ON	2-4	OFF	ON
MFT 1-3	m13c14	OFF	1-4	ON	1-3
MFT 2-3	m23c14	OFF	1-4	ON	2-3
MFT 1-3	m13c24	OFF	2-4	ON	1-3
MFT 2-3	m23c24	OFF	2-4	ON	2-3
SFT 1-4 + MFT 1-3	m13s14	ON	1-4	ON	1-3
SFT 1-4 + MFT 2-3	m23s14	ON	1-4	ON	2-3
SFT 2-4 + MFT 1-3	m13s24	ON	2-4	ON	1-3
SFT 2-4 + MFT 2-3	m23s24	ON	2-4	ON	2-3

Efficiency	SFT-B	MFT-B	Ideal
ϵ_{s14}	1-4	OFF	1
ϵ_{s24}	2-4	OFF	1
$\epsilon_{m13r12c14}$	1-4	1-3	1
$\epsilon_{m13r23c14}$	1-4	1-3	1
$\epsilon_{m23r12c14}$	1-4	2-3	0
$\epsilon_{m23r23c14}$	1-4	2-3	1
$\epsilon_{m13r12c24}$	2-4	1-3	1
$\epsilon_{m13r23c24}$	2-4	1-3	1
$\epsilon_{m23r12c24}$	2-4	2-3	0
$\epsilon_{m23r23c24}$	2-4	2-3	1
σ_2/σ_1			1

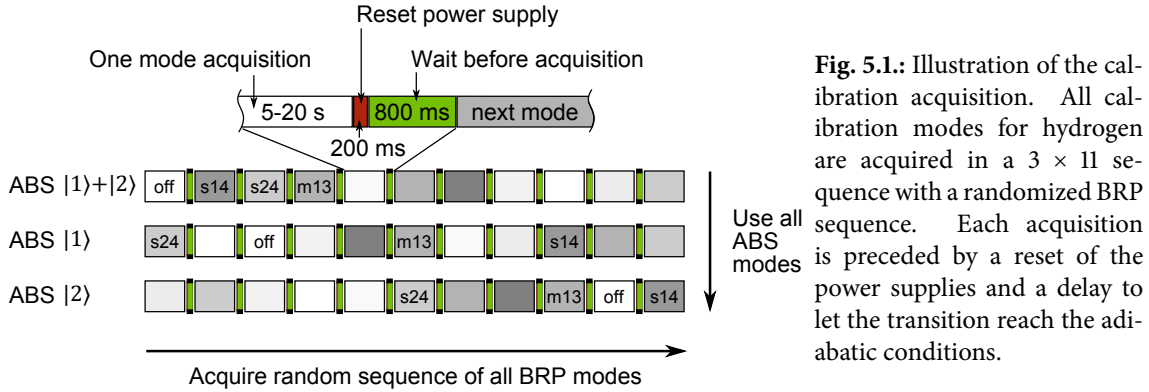
Table 5.2.: The BRP calibration efficiencies for hydrogen are composed of 10 transition efficiencies and the sextupole transmission ratio σ_2/σ_1 . Each efficiency is only valid for a specific magnetic field setting on both the SFT and MFT transition units.

5.1.2. Acquisition Procedure

In the acquisition procedure all signals necessary for the calibration are measured sequentially. For hydrogen this means acquiring all 11 BRP modes of Table 5.1 for each ABS injection mode. For hydrogen the ABS has three possible injection modes: $|1\rangle + |2\rangle$ with ABS MFT switched off (mode rfoff), $|2\rangle$ with the ABS mode m23m12 and $|1\rangle$ with the ABS mode m23. To avoid any systematic

error resulting from the switching order, the BRP acquisition sequence is randomized for each ABS mode.

The power supplies for the coils have a hysteresis and might set a different value depending on the previous setting. This effect is avoided by resetting the output value to zero before setting the required current value. The reset lasts for 200 ms and precedes the activation of the mode. Additionally, the power supplies for the magnetic field coils and the rf emitters need time to reach their value set by the DAC. Therefore, each switching of a mode is followed by a 800 ms delay to let the HFT reach the adiabatic condition. The acquisition of the signal time spectrum starts after that delay. An illustration of the calibration acquisition sequence with the delay time is shown in Fig. 5.1.



The calibration requires the measurement of all 33 signals preferably with the smallest possible statistical error, meaning a sufficient acquisition time. However, the ABS can not be guaranteed to deliver an absolute stable intensity over hours and any change in intensity will introduce a systematic error in the efficiencies. To avoid this problem the sequence of the 33 hydrogen signals (3×11) is acquired multiple times using a short acquisition time of typically 10 chopper cycles (≈ 5 seconds). This minimal full acquisition of all calibration signals takes about 3.5 minutes and is called a calibration cycle. The acquisition of a calibration cycle can be repeated as many times as necessary to reach a sufficient error for the efficiencies. By creating signal replicates, the calibration cycle measurements not only solve the ABS stability problem, but also the calibration results can be verified online during the calibration routine and can be interrupted at any time. A typical calibration for hydrogen with errors of less than 1% requires 50×33 measurements with a 10 cycles acquisition and lasts about 3 hours.

For the calibration analysis it is possible to either average all identical modes and thus reduce the number of signals to $n = 33$ for hydrogen, or keep all measured modes as they are and fit the efficiencies over all measured signals (for example 50×33 signals). The average method provides the same signal quality and error as if the acquisition was done only once with a corresponding high chopper cycle and thus a longer acquisition time. However, the advantage is that any ABS instability or slow intensity drift is averaged out. For the average method the mean μ_n and the variance δ_n^2 of a mode n are calculated with a weighted average of the same signals S_i ; $i = 1, 2, \dots, m$ [137]:

$$\mu_n = \frac{\sum_{i=1}^m S_i W_i}{\sum_{i=1}^m W_i} \quad \text{and the variance} \quad \delta_n^2 = \frac{1}{\sum_{i=1}^m W_i} \quad \text{with the weight} \quad W_i = \frac{1}{\delta_i^2}. \quad (5.1)$$

The averaging of signals before fitting should be avoided in general as it might hide the true signal variance to the fitting algorithm [138]. However, the averaging of replicates still provides a reliable variance as long as the variance can be considered Gaussian and that the measured signals replicates have an approximate normal distribution. This is typically the case with an acquisition of 20 to 30 calibration cycles using 10 chopper cycles. Reducing the chopper cycles, however, will increase the variance of the replicates and will require more cycles if the averaging method is used.

Fitting directly all acquired signals with the implemented algorithm is also possible, but the use of large matrices in the order of 50×33 will significantly increase the required computational time. For example, with 35 calibration cycles the direct fit method will converge in about one hour while the fitting of the averaged 33 signals converges within a few seconds¹. The numerical results between both methods are identical within the error. The direct fit results in a higher χ^2 value but in lower errors ($\approx 35\%$ lower for the direct fit). The results displayed in this work and used for the polarization measurements use the averaging method.

5.2. Tuning of the Transitions

As seen in the slow control Sec. 4.7, the HFTs are controlled by four parameters: the amplitude and frequency of the rf and the homogeneous and gradient magnetic field coil currents. Those four values are controlled by voltages from the DAC. A typical tuning procedure consists of selecting an rf amplitude and frequency and also a fixed value for the gradient field current. The tuning procedure is a scan of the homogeneous magnetic field current to find the transition resonance. This procedure can locate the SFT transitions directly as the SFT single photon transitions are unambiguous. However, the MFT is composed of 2 (3) sub-transitions for hydrogen (deuterium)² and the tuning procedure requires either the knowledge of the beam population distribution or the help of the SFT transition to distinguish the MFT sub-transitions. The procedure used to tune all transitions for hydrogen is as follows:

- Tuning of the BRP SFT transition directly by scan. The transition does not require additional knowledge.
- Tuning of the ABS MFT transition with the help of the BRP SFT.
- Tuning of the BRP MFT with the help of both the ABS MFT and the BRP SFT.

5.2.1. Tuning of the BRP SFT

The SFT rf frequency is matched to the cavity resonance with the VCO. The cavity resonance is reached when the pick-up amplitude is maximal ($f = 1447$ MHz). The rf amplitude is set to 5 mW which is the maximal input for the amplifier. Initially the gradient field coil is typically set to 1 A. The SFT transitions can be reached with a negative or positive gradient. Scanning the homogeneous field from zero to higher values will reveal the two SFT resonances. Taken from Fig. 2.5b, the SFT 1-4 transition occurs at a low magnetic field and the SFT 2-4 transition requires a stronger magnetic field. A scan of the homogeneous magnetic field is shown in Fig. 5.2. The two SFT transitions are clearly separated and their identification is unambiguous. The scan is performed with the ABS mode off which injects the states $|1\rangle + |2\rangle$. The atomic gas in the storage cell is therefore composed ideally of those two states. When the SFT 1-4 (2-4) reaches the transition condition, the populations in the state $|1\rangle$ ($|2\rangle$) are exchanged with the populations of state $|4\rangle$. Therefore, because of the spin selection in the sextupole magnets the SFT transitions effectively suppresses up to half of the signal. The two resonances have not the same minimum and the signal is reduced by less than half. This effect is not due to the transition efficiencies but to the non ideal and inhomogeneous hyperfine state populations distribution inside the storage cell. This effect is due to spin-exchange and relaxation and will be discussed in chapter 6.

In general the strength of the gradient field does not affect the transition efficiency as long as all atoms experience the transition condition. A stronger gradient has the effect of widening the transition resonance forming a plateau and leading to a more stable efficiency. The reason is that

¹PC with Intel CPU Core2 Duo @3.00GHz, 4 GB memory running on Linux kernel 2.6.31 (SuSE 11.2 32 bit).

²The hydrogen MFT is a two photon transition (3 for deuterium), see Sec. 2.4.3.

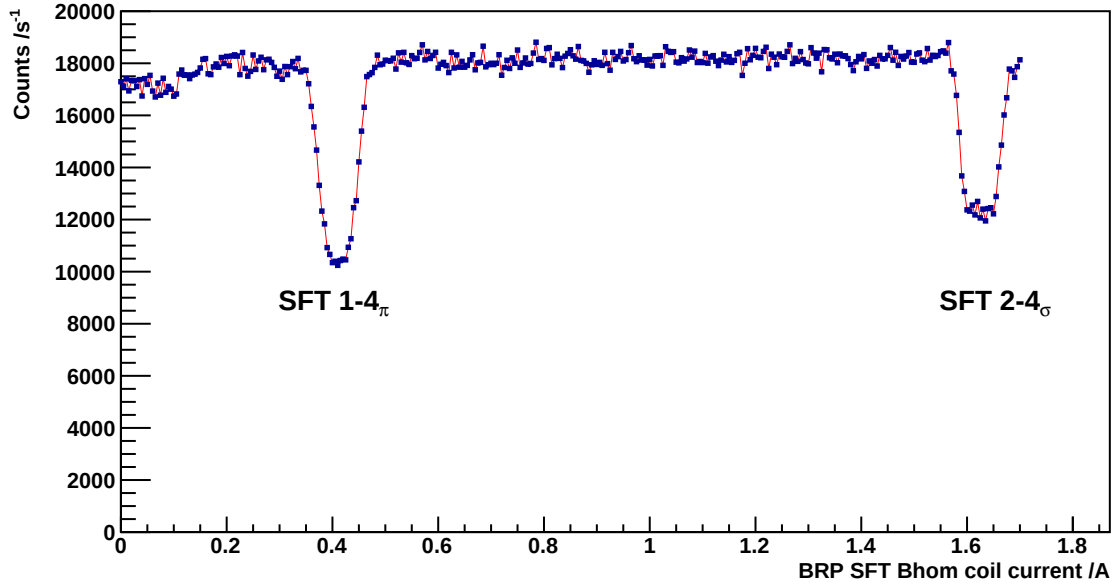


Fig. 5.2.: Scan of the homogeneous magnetic field of the BRP SFT. The frequency, amplitude and gradient field are fixed during the scan ($f = 1447$ MHz, VCO amplitude = 5 mW, $I_{\text{gradient}} = 0.36$ A).

a small parameter shift, e.g., of the frequency or coil current, will shift the transition within the plateau and keep the efficiency unchanged. The BRP SFT 1-4 transition exhibits a better efficiency for lower gradient fields; however, the SFT 2-4 efficiency is unaffected by the gradient strength. The selected low gradient coil current of 0.6 A used for Fig. 5.2 narrows the resonance conditions and the transition will show a higher sensitivity to any parameter variation. A scan of the homogeneous magnetic field with different ABS injection modes is provided in Fig. C.3.

5.2.2. Tuning of the ABS MFT

The injected hydrogen states listed in Table A.2 are chosen by the MFT by selecting either the single 2-3 transition or the combined 2-3 and 1-2 transitions. Because the MFT 1-2 sub-transition does only affect the population of states with the same electron spin, the intensity after the sextupole magnets does not change. The ABS compression tube is therefore not sensitive to the 1-2 transition. The tuning of the ABS MFT requires the use of the BRP to differentiate the transition regions of m23 and m23m12 for the injection of states $|1\rangle$ and $|2\rangle$ respectively. The frequency and the gradient field are fixed ($f = 66$ MHz, $I_{\text{gradient}} = 0.75$ or 1.5 A) and the homogeneous field is scanned to locate the transition resonance regions. A signal drop in the BRP indicates the effect of a transition. The scan is performed once with the BRP SFT 1-4 and once with the BRP SFT 2-4. A reference scan without SFT is also performed. Figure 5.3 shows the three scans of the ABS MFT with the effect of the BRP SFT transitions. The scans are performed with two different gradients.

The BRP SFT selectively removes the states $|1\rangle$ or $|2\rangle$ from the sampled beam coming from the storage cell and is therefore able to identify the ABS MFT sub-regions. The BRP SFT 1-4 (2-4) transition reveals the ABS MFT m23 (m23m12) transition. The best homogeneous magnetic field settings for m23 and m23m12 are at the minimum of each region. A strong gradient widens the transition regions and separates the sub-transitions further apart. This effect can be seen in the lower panel of Fig. 5.3.

For the low gradient (top panel in Fig. 5.3), the region of the combined transitions m23m12 is narrow and does not reach much into the m23 region although it is near to it. The reason is that the low gradient can not (or barely) reach both m23 and m12 transitions within the rf region of the MFT coil. Therefore, the efficiency of m23m12 is lower than the m23 transition. A good separation

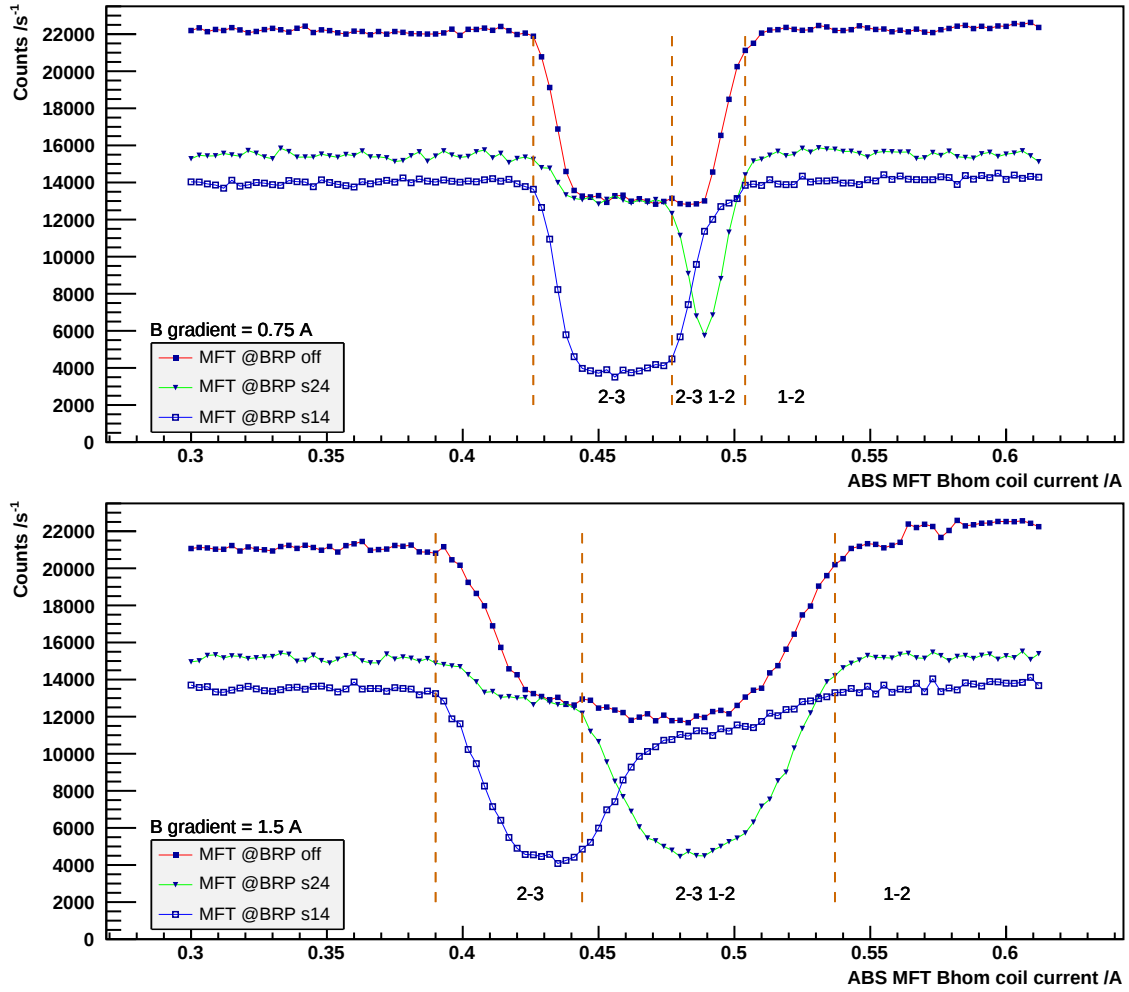


Fig. 5.3.: Scan of the homogeneous magnetic field of the ABS MFT using the BRP SFT to differentiate the two transition regions m23/m23m12. The regions of the sub-transition are marked with vertical dashed lines. The top graph shows the transition regions with half the gradient compared to the lower graph. The scans are performed with a positive gradient. A negative gradient can only inject the state $|1\rangle$ as the m23 sub-transition occurs after the m12 in any magnetic field setting.

between the sub-transitions m12 and m23 is required to inject the state $|1\rangle$ only, in which case the transition m12 starting at a higher magnetic field has to be avoided. Even though the top panel of Fig. 5.3 scan seems to provide less separation of the transitions, the m23 transition has a larger plateau and a better efficiency due of the better spacial separation of the sub-transitions provided by the lower gradient. The low gradient setting is therefore used to inject the state $|1\rangle$ with the m23 transition.

In the stronger gradient case (bottom panel in Fig. 5.3), the m23m12 region is better defined compared to the lower gradient. The position of the minimum is not only clearly separated from the m23 position but the m23 transition does not reach so much into the m23m12 region. However, due to the lower spacial separation of the sub-transitions with the stronger gradient setting, the plateau and efficiency of the m23 transition is reduced. This gradient is therefore used to inject the state $|2\rangle$ used only during calibration.

5.2.3. Tuning of the BRP MFT

As with the ABS the BRP MFT requires the help of another transition to separate the MFT sub-transitions. In addition the cross-talk with the SFT has to be taken into account. Two methods are

used to tune the MFT. The first uses the SFT transition to change the hyperfine population before the MFT. However, the SFT 1-4 and 2-4 setting will only tune the MFT with respect to their cross-talk mode. That is, the modes $m_{xx}c_{14}$ are tuned with the SFT 1-4 and the modes $m_{xx}c_{24}$ are tuned with the SFT 2-4 (the m_{xx} transition means both m_{23} and m_{13}). The second method uses the two possible ABS single state injection modes to find the sub-transition regions. With this method the cross-talk calibration setting can be set to either value c_{14} or c_{24} and the scans are performed for both modes. Figure 5.4 shows the magnetic field scans of the BRP MFT using both methods to tune the modes $m_{23}c_{14}$ and $m_{13}c_{14}$.

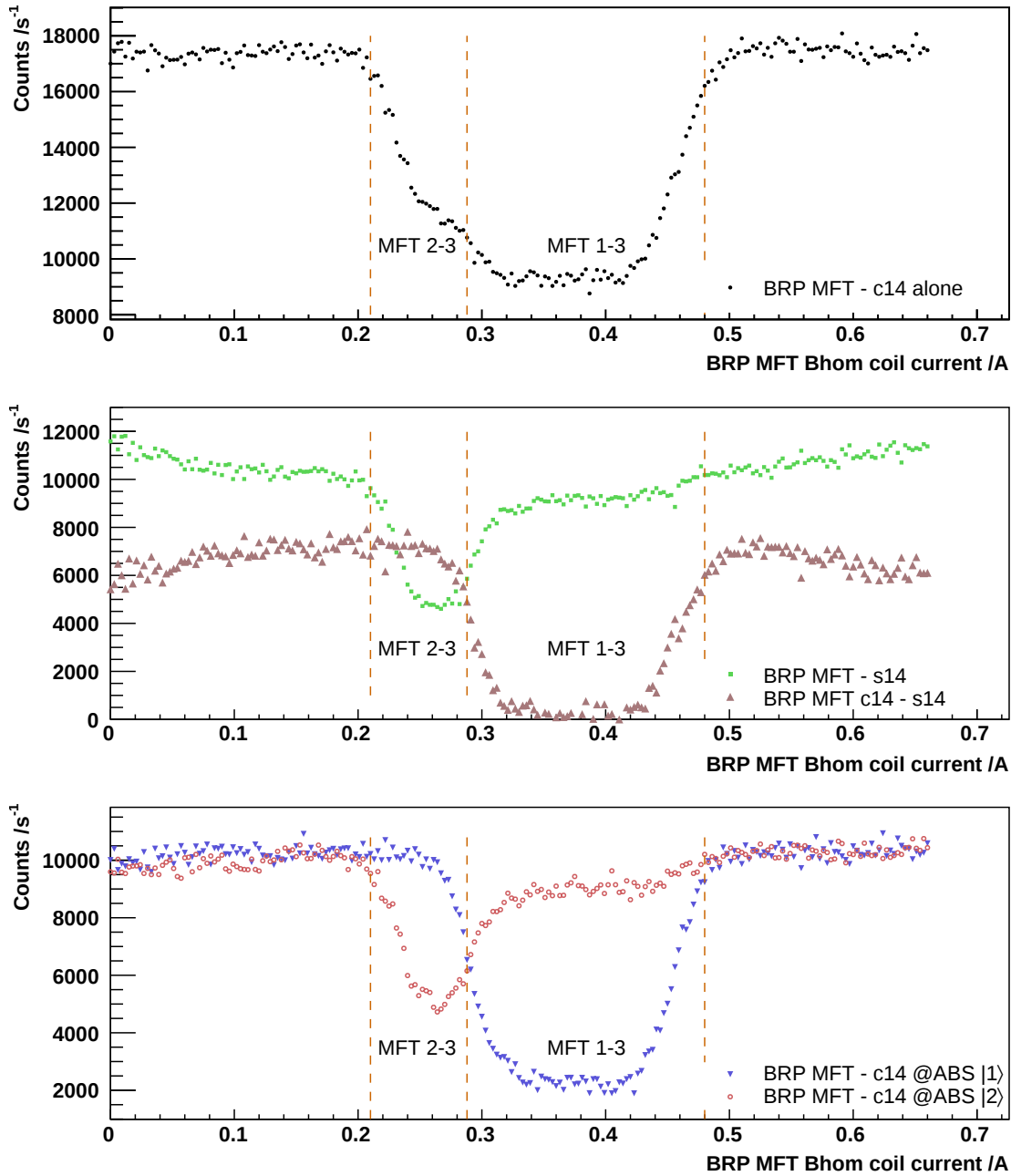


Fig. 5.4.: Scans of the homogeneous magnetic field of the BRP MFT with the c_{14} magnetic field setting. The top scan shows the MFT transition with the SFT off and the ABS MFT off (injection of states $|1\rangle + |2\rangle$). This scan alone can not differentiate the MFT sub-transitions. The middle scan is performed with the SFT 1-4 switched on, the second data set (triangles markers) shows the difference between the MFT scans with SFT 1-4 switched on and off. The bottom scans are performed with the ABS injection modes $|1\rangle$ and $|2\rangle$. The vertical dashed lines indicate the regions of the active sub-transitions.

Using the tuning method with the SFT 1-4 the principle is to acquire first an MFT homogeneous magnetic field scan without the SFT (mxxc14) and second a scan with the SFT 1-4 switched on (mxxs14). The best settings for the mode m23c14 are provided by the mxxs14 scan because the SFT 1-4 suppresses the state $|1\rangle$ only state $|2\rangle$ remains in the beam. The best setting for the MFT 2-3 transition is found at the minimum of the scan. The best m13c14 mode is found by plotting the difference mxxc14–mxxs14. The two curves are shown in the middle plot of Fig. 5.4. The MFT 1-3 where both sub-transitions m12 and m23 are active exhibit a plateau and begins at a higher magnetic field than the MFT 2-3 transition. The reason for the MFT 1-3 plateau is illustrated in Fig. 5.5 and is explained in the next paragraph.

For the MFT two (three for deuterium) sub-transitions must occur within the rf field region inside the few centimeters of the coil. When the MFT 1-3 conditions are met, the position of the magnetic fields for the two sub-transitions are both inside the rf region of the MFT rf coil. When the homogeneous magnetic field is increased, the conditions for the two sub-transitions are shifted along the beam axis. The m13 transition is active as long as both sub-transitions are kept inside the rf region. On the other hand, the m23 transition can only be shifted as long as the m12 is kept outside the rf region.

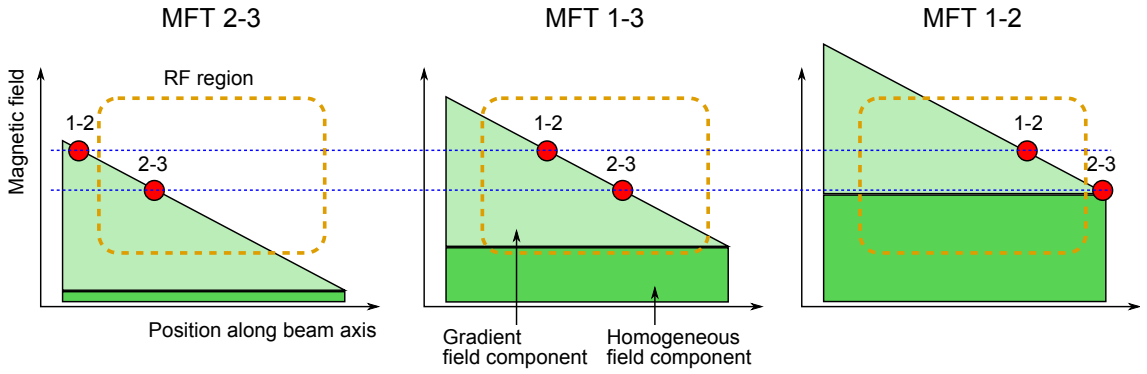


Fig. 5.5.: Effect of the homogeneous magnetic field to the MFT sub-transitions. The separation of the two sub-transitions is dictated by the fixed gradient (and also the fixed rf frequency) and the value of the magnetic field is given by the frequency (see Fig. 2.5) and is marked by the two horizontal dashed lines. The magnetic field conditions for the transition are symbolized by a circle. An increase of the homogeneous component of the magnetic field has the effect of shifting the transition conditions along the beam axis. A strong gradient will reduce the spacial separation of the sub-transitions and therefore reduce the plateau of a single sub-transition. In the same way, a strong gradient increases the plateau of a multiple transition. A very low gradient, however, will reduce the efficiencies of a multiple transitions when the sub-transitions are pushed too close to the edge of the rf field.

With the ABS tuning method the same scan mxxc14 is performed once with the injection of state $|1\rangle$ and then with the injection of state $|2\rangle$. The different populations in the cell will then reveal the MFT 2-3 and MFT 1-3 regions. If the extracted beam from the cell is mainly populated with atoms in the state $|1\rangle$, the MFT 1-3 transition will remove most atoms from the beam. This will reduce the signal intensity and create a minimum at the optimal MFT 1-3 setting. The sub-transition m23 will ideally have no effect on the signal when the state $|1\rangle$ is injected, but will display a minimum when the state $|2\rangle$ is injected. The bottom panel in Fig. 5.4 shows the two curves with the different ABS injections and permits one to locate the two transitions optima. Both complementary tuning methods reveal the same information (see Fig. C.4 for the tuning with the c24 SFT settings).

5.3. Correction Factors

5.3.1. H₂ Background from the TGA Chamber

The states deflected by the sextupole magnets and the recombined H₂ molecules from the storage cell increase the H₂ partial pressure in the TGA and sextupole chambers. Since this pressure is larger than in the BRP detector chamber, there is a net H₂ flow toward the BRP QMA. H₂ molecules are partially dissociated by the QMA ionizer (in the order of 1% [85]) and therefore the molecular beam will artificially increase the count rate of mass 1 in the BRP. This systematic error is corrected by measuring the relative amount of the BRP signal generated by the H₂ molecules coming from the TGA chamber. The measurement is done with the help of the beam shutter in the TGA chamber. The principle is to measure the BRP signal at various injection intensities with the beam shutter open and closed. When the beam shutter is closed all atoms entering the TGA chamber will hit the beam shutter and recombine. In this case the measured BRP signal originates from the partial dissociation of H₂ molecules coming from the TGA chamber. The change of magnetron output power, and thus the degree of dissociation, is used to vary the ABS intensity. The different output power settings used for this measurement are approximately 50%, 75%, and 100%. Additionally, the ABS MFT can be switched on or off leading to two injection intensities per power setting for a total of 6 different intensities. The low count rate measured with the closed shutter is acquired with a 1000 cycles average to reduce the statistical error. The open position is acquired with 10 cycles before and after the closed position. For each injected intensity the measurement time is about one hour. The error is calculated using the observed variance, as described in Sec. 4.6.3. Figure 5.6 shows the correlation between the injected intensity with the beam shutter open and the background signal with the beam shutter closed.

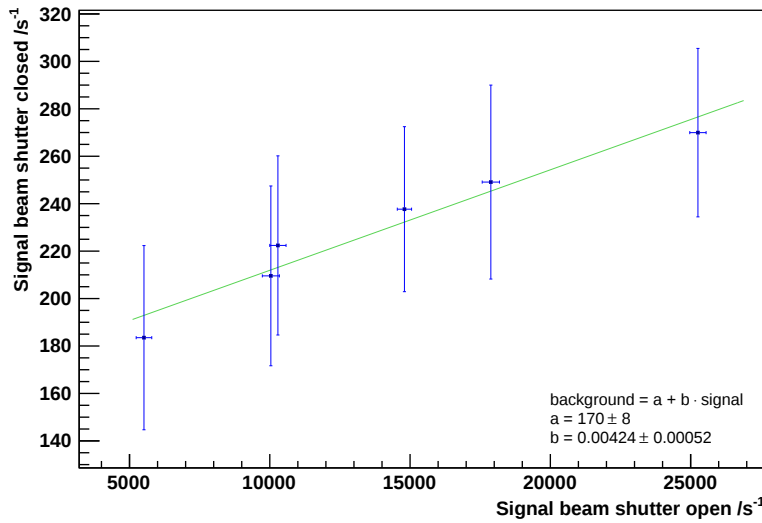


Fig. 5.6.: Signal generated by the H₂ background from the TGA chamber. The molecular H₂ flow from the TGA chamber partially dissociates in the QMA ionizer and generates a background signal for mass 1. The measured background depends only on the beam intensity coming from the cell. Measured with 50%, 75%, and 100% magnetron power combined with two ABS injection states.

The background is described with a linear function

$$\text{background} = a + b \cdot \text{signal}. \quad (5.2)$$

The parameters a and b are fitted to the data with:

$$a = 170 \pm 8 \quad (5.3)$$

$$b = 0.00424 \pm 0.00052. \quad (5.4)$$

The background intensity is not zero without ABS injection ($a = 170$). This might be explained by a higher partial pressure of hydrogen or water in the target chamber and TGA chamber than in the BRP chamber. The background is a function of the intensity of the beam from the storage cell and

does not depend on the BRP settings. During a polarization (or calibration) measurement cycle the BRP count rate varies with each HFT setting, the background (5.2) is calculated with the BRP off (rffoff) mode within the measurement cycle. The same background value is then subtracted from all signals belonging to this measurement cycle. The correction error is propagated to the signals with:

$$\delta_{bkg}^2 = \delta_a^2 + (S_{rffoff} \cdot \delta_b)^2 \quad (5.5)$$

$$\delta_{Si(new)}^2 = \delta_{Si}^2 + \delta_{bkg}^2 \quad (5.6)$$

5.3.2. Mass Spectrometer Emission Current

The signal amplitude measured by the QMA depends on the emission current of the ionizers filament. A higher current will increase the signal. The emission current is typically operated close to 1000 μA and is stable over a period of minutes, but can vary up to 2-4% within an hour and up to 10% during a day. Specifically, a rise in room temperature will reduce the emission current. This variation is not a problem as long as the current is stable during a measurement cycle. This is usually the case because even a long polarization cycle takes less than 2 minutes and a calibration cycle typically requires 3-4 minutes or a maximum of 10 minutes. However, at longer acquisition times the signals are distorted if the current changes during a cycle. Thus, the variation of the emission current induces a systematic error. Figure 5.7 shows the raw count rate related to the emission current measured directly without chopper.

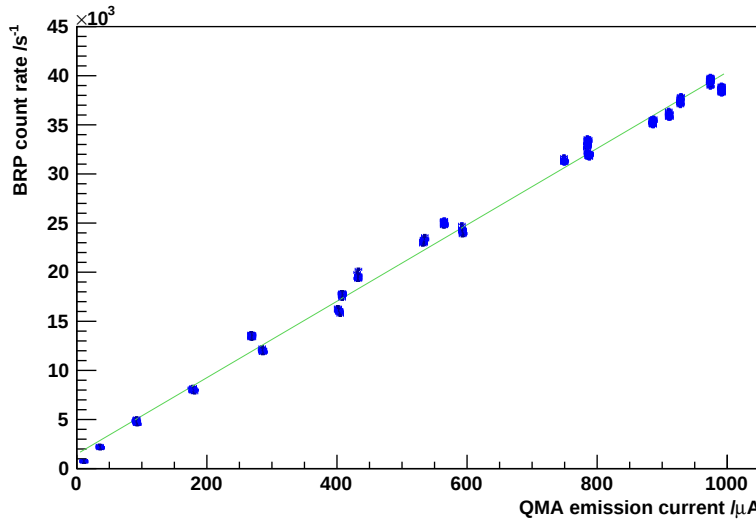


Fig. 5.7: Linear dependency of the BRP count rate on the emission current. The count rate and the emission current can take up to 10-20 minutes to reach stable values when the emission current is changed, specially when the current is increased. Therefore, two measurements carried out with the same emission current at different times might result in different count rates, even if the signal is stable.

About 10-15 measurements are performed per emission current setting and the current values are changed in an alternating increasing and decreasing order. The measured values require up to 10-20 minutes to fully stabilize; however, a short measurement of all points is preferable to avoid variations in the vacuum conditions or of the ABS intensity. For this measurement a delay of 2 minutes is introduced after setting the emission current and before measuring the count rates. This short stabilization time results in different count rates for a similar emission current. The count rates S_i are clearly linear with the emission current I_{em} and can therefore be normalized:

$$S_{i(norm)} = S \cdot \frac{1000}{I_{em}} \quad (5.7)$$

The emission current is read by the CAMAC ADC module (see Sec. 4.6.2) for each time spectrum acquisition. The normalization is performed in respect to the maximal emission current of 1000 μA (the input range of 0-10 V corresponds to an emission current of 0-1000 μA). An error of 50 mV

($\delta_{I_{em}} = 5\mu\text{A}$) is assumed for the polarization and calibration analysis. The emission current error $\delta_{I_{em}}$ is propagated to the signal with

$$\delta_{S_i(norm)}^2 = S_{i(norm)}^2 \cdot \left[\left(\frac{\delta_{S_i}}{S_i} \right)^2 + \left(\frac{\delta_{I_{em}}}{I_{em}} \right)^2 \right] \quad (5.8)$$

5.4. Implementation of the Fitting Algorithm

The two nonlinear least square fit algorithms described in Sec. 3.4 (Gauss-Newton and Lagrange multipliers) have been implemented in a C++ program to fit the unknown calibration values to the data taken for the calibration. In the model the ABS and BRP are expressed as a succession of transition matrices (2.75) and vectors (2.85) for the sextupole magnets. The transitions can be switched on or off leading to $N_{ABS} \cdot N_{BRP}$ different signals each modeled by a function $g_i = \sum_k M_{ik} I_k = S_i$. Each signal is composed of a combination of 4 (6) hyperfine state intensities I_k for hydrogen (deuterium). As seen in Sec. 3.2, for each BRP mode the effect of the n active adiabatic transitions with efficiencies ϵ_l and of the sextupole magnets with transmission probabilities σ_j is described by one row of the measurement matrix $M_{ik} = \sum_b \sigma_b \prod_n T_{bk}^n$. In the algorithm the signals S_i are modeled with $g_i(x; \beta_1, \beta_2, \dots, \beta_n)$ functions, with β being the vector of unknown parameters $\beta = (\epsilon_l, \sigma_j, I_k)$. For both algorithms the starting values for the injected intensities are a simulation of ABS injection state populations scaled to match the measured BRP rfoff signal. A good guess for the intensities will help the algorithms to converge and also improve the speed of convergence.

The Gauss-Newton algorithm modifies β to find the best $\mathbf{g}(x; \beta)$ to match the vector of signals $\mathbf{S}$. The algorithm inputs are $\mathbf{S}$, $\mathbf{g}(x; \beta)$ and β set to first estimates (the ideal efficiencies). The partial derivatives for the Jacobi matrix are solved numerically with

$$\frac{\partial g}{\partial x_i}(\beta_1, \dots, \beta_n) = \frac{g(\beta_1, \dots, \beta_i + h, \dots, \beta_n) - g(\beta_1, \dots, \beta_n)}{h} \quad (5.9)$$

where h is the difference quotient set to a small value ($h = 10^{-5}$). The BRP model is nonlinear, but because each unknown enters linearly in $g(x; \beta)$, the numerical derivatives produce exact solutions. The χ^2 value is calculated after each iteration and the process is stopped when the difference to the previous iteration is $\Delta\chi^2 < 10^{-6}$.

The Lagrange multipliers algorithm minimizes a vector of functions $f_i(\mathbf{x}, \boldsymbol{\eta}) = 0$ (3.47) which combines the model and the signals. The algorithm treats the observable $\boldsymbol{\eta}$ and the unknown $\mathbf{x}$ in the same way and tries to minimize the residual

$$f_i(\mathbf{x}, \boldsymbol{\eta}) = g_i(\mathbf{x}) - \eta = 0.$$

The first approximation for the observable $\boldsymbol{\eta}$ are the measured signals $\boldsymbol{\eta}_0 = \mathbf{S}$ and the first estimate for the unknown $\mathbf{x}_0$ are the ideal efficiencies. The two Jacobi matrices (3.51) are calculated according to (5.9). In addition to the values provided for the Gauss-Newton algorithm, $f_i(\mathbf{x}, \boldsymbol{\eta})$ and the vector of corrected signals $\boldsymbol{\eta}$ must be provided to the Lagrange algorithm.

For both algorithms the signal is weighted by the observed variability (4.2). The signal variation is used to define the covariance matrix $\mathbf{C}_S$ (3.15) and the weight matrix $\mathbf{W}_S = \mathbf{C}_S^{-1}$. This weighting method is only valid if the errors are Gaussian which we can assume for the count rate. Both algorithms return the covariant matrix of the efficiencies given by the equations (3.44) and (3.61). The results for the efficiencies are identical between the two algorithms, however, the covariant matrices and corresponding χ^2 values are not. The reason is that the Lagrange algorithm treats the signals as observables with errors and the χ^2 to be minimized is different. Nevertheless, in both cases the combination of the covariant matrix and the quality of fit χ^2 lead to the same errors.

5.5. Results of the Calibration

The calibration measurement for hydrogen typically requires > 25 calibration cycles of 33 signals as described in 5.1.2 to reach a statistical error below 2%. The calibration presented here was performed with 35 calibration cycles. A calibration cycle is comprised of 33 BRP signals using the 3 ABS injection modes times 11 BRP settings. Each BRP mode is acquired over 10 chopper revolutions. The calibration results calculated with the Lagrange Multipliers fitting algorithm are shown in Table 5.3. Before fitting all replicate modes are averaged according to Eq. (5.1). The signal errors are used to weight the modes in the algorithm.

The fitting algorithms for the calibration calculate both the intensities and the efficiencies. The form of the resulting covariance matrix of the unknown C_x depends on the order of the unknowns in the vector $\mathbf{x}$. Both implemented algorithms produce a covariance matrix:

$$C_x = \begin{pmatrix} C_I & C_{I,\epsilon} \\ C_{I,\epsilon} & C_\epsilon \end{pmatrix}. \quad (5.10)$$

The matrix C_ϵ is used to calculate the systematic uncertainties of the polarization as described in Sec. 3.2.2. The statistical errors in Table 5.3 are calculated with

$$\delta_{\epsilon_i,stat} = \sqrt{\chi^2(i)C_{\epsilon_{ii}}} \quad (5.11)$$

and are of statistical nature. The final χ^2 is taken from the last iteration of Eq. (3.59).

Table 5.3.: BRP calibrated efficiencies for hydrogen. The model (3.8) is fitted to the data with the Lagrange Multipliers algorithm. The calibration data consist of 35 calibration cycles of 33 BRP signals using 3 ABS modes. The errors are statistical.

Efficiency	SFT-B	MFT-B	Ideal	Value	Error
ϵ_{s14}	1-4	OFF	1	1.0022	± 0.0089
ϵ_{s24}	2-4	OFF	1	1.005	± 0.012
$\epsilon_{m13r12c14}$	1-4	1-3	1	0.993	± 0.010
$\epsilon_{m13r23c14}$	1-4	1-3	1	0.937	± 0.011
$\epsilon_{m23r12c14}$	1-4	2-3	0	0.0665	± 0.0079
$\epsilon_{m23r23c14}$	1-4	2-3	1	0.850	± 0.010
$\epsilon_{m13r12c24}$	2-4	1-3	1	1.014	± 0.011
$\epsilon_{m13r23c24}$	2-4	1-3	1	0.951	± 0.011
$\epsilon_{m23r12c24}$	2-4	2-3	0	0.0959	± 0.0073
$\epsilon_{m23r23c24}$	2-4	2-3	1	0.890	± 0.010

The SFTs are operating at 100% efficiency, the MFT 1-3 transitions are also running at a high efficiency above 90%. The MFT 2-3 transitions could not be tuned to efficiencies above 90%. However, this lower efficiency does not reduce the BRP precision because the systematic error of the polarization depends only on the errors of the efficiencies. Furthermore, the polarization measurements do not require all 11 modes and a typical polarization measurement is acquired without the MFT 2-3 transition³.

Only the single unknown ratio σ_2/σ_1 of the sextupole transmission probabilities is required to describe the sextupole system. However, the fitting algorithm will not converge when the ratio σ_2/σ_1 is added to the unknown parameters. The reason is that the effect of the sextupole magnets

³The 2-3 transition is not required for the polarization measurement but is required for the calibration to obtain an overdetermined system.

is too small or absent on some signals leading to a non-invertible degenerated Jacobian matrix in Eqs. (3.8) or (3.42). For example, the mode m13s24 ideally converts a beam composed of the state populations N_1 and N_2 into the populations N_3 and N_4 . This converted beam will ideally be fully defocused by the sextupole magnets regardless of the ratio σ_2/σ_1 . Such a noneffective parameter in the model creates a row of zeros in the Jacobian matrix, and the matrix can therefore not be inverted.

The ratio σ_2/σ_1 can be calculated by fitting the model (3.1) to the data taken during a polarization measurement. Each polarization measurement acquired with at least 5 modes can be used to fit σ_2/σ_1 in addition to the intensities. However, due to the small effect of the ratio, the fitted value σ_2/σ_1 will have a large variation. This large variation for each fit can be overcome by fitting with multiple measurements and extracting the mean. The fitted σ_2/σ_1 values calculated with over 3000 polarization cycles and varying chopper cycle lengths are plotted in the histogram in Fig. 5.8. The histogram is fitted with a Gaussian to extract the resulting σ_2/σ_1 ratio. The result is

$$\sigma_2/\sigma_1 = 0.9973 \pm 0.0005. \quad (5.12)$$

The large number of measurements reduced the error of the mean of the Gaussian. Since the error is two orders of magnitude smaller than the ones for the efficiencies, it is not included in the systematic error of the polarization.

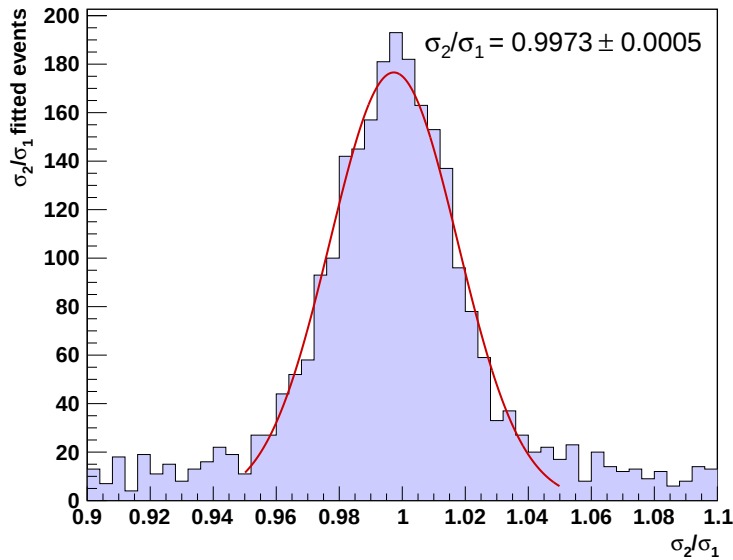


Fig. 5.8.: Ratio σ_2/σ_1 fitted over (>3000) polarization cycles.

6. MEASUREMENTS

6.1. Results of the Polarization Measurements

6.1.1. Measurement Procedure

The BRP measures the relative hyperfine state populations of a hydrogen (deuterium) atomic beam sampled from the storage cell. The atomic polarization is calculated using the hyperfine state occupancy together with the magnetic field strength and the polarization Eqs. (2.51) (Eqs. (2.55) for deuterium)¹. The BRP signals are a linear combination of the hyperfine state population intensities I_a and are described by the measurement matrix (Sec. 3.2):

$$S_i = \sum_a M_{ia} I_a; \quad \text{with} \quad M_{ia} = \sum_b \sigma_b \prod_n T_{ba}^n. \quad (6.1)$$

The variables of the measurement matrix M_{ia} are determined during the calibration. The system of equations (6.1) can be solved for the intensities I_a if the number of acquired signals is equal to the number of unknown intensities. Therefore, at least 4 (6) signals generated with different combinations of high-frequency transitions are necessary to measure the polarization for hydrogen (deuterium).

As in the calibration procedure, the acquisition order is randomized for each measurement to avoid any systematic error caused by the order of measurement in the sequence. The signals acquired for one polarization measurement are arranged into a *polarization run*. The three different polarization sequences for a run used during the polarization measurement are listed in Table 6.1.

Number of signals	Used transition modes
5	rfoff s14 s24 m13s14 m13s24
7	rfoff s14 s24 m13s14 m13s24 m13c14 m13c24
11	all BRP modes from Table 5.1

Table 6.1.: Transitions used for the different polarization runs for hydrogen

For one measurement the slow control system sets the hardware and acquires all modes of a run in sequence. The offline software is then used to calculate the hyperfine state intensities using Eq. (3.8) and the polarization via Eq. (3.13). The same program is used to calculate the polarization based either on the online or the offline signals. The difference is that for the processing online signals, a simplified evaluation of the time spectrum is used, while the offline signals are based on the analysis of the full time spectrum; thus, permitting to evaluate the error and to apply the corrections explained in Sec. 5.3. Also a shift of the time bins due to a wrong trigger event can be corrected in the offline analysis.

6.1.2. Uncertainties of the Measurements

The systematic errors of the polarization are based on the errors of the transition efficiencies (see Sec. 3.2.2) and thus are limited by the statistical accuracy reached during the calibration. A statistical

¹The analysis software uses the matrix notation (3.13).

error of 1% for the efficiencies typically translates into a systematic error of $\Delta P_z = 0.005$ for the polarization. Because the polarization depends on the magnetic holding field, its uncertainty has to be taken into account for the systematic error of the polarization. This uncertainty, however, is not related to the BRP measurement and is not considered here. Additionally, the inhomogeneity of the field along the storage cell also induces a systematic error. However, because of the low holding field used for the spin-filtering studies the uncertainties of the magnetic holding field will have a negligible impact on the polarization.

The statistical error of the polarization is dictated by the uncertainties of the signals and the quality of the fit used to calculate the hyperfine state intensities (Sec. 3.2.1). A higher signal intensity or a longer acquisition time will reduce the statistical error of the polarization.

The following measurement has been performed to identify the expected standard deviation based on the acquisition time required for one polarization measurement. The duration required for a polarization measurement is varied by selecting different chopper cycles (1, 2, 5, 10, 20, 35) and using the three sequences listed in Table 6.1. The polarization is measured multiple times for each of the 18 different cycle/sequence combinations and the resulting value is plotted in a histogram. The distribution of the polarization is analyzed by fitting the histograms with a Gaussian. The resulting standard deviation σ is plotted against the duration of the measurement. The indicated error on the deviation is the error of the fit. A sequence with more modes requires more time to complete for the same number of chopper cycles. However, different sequences measured for the same duration should provide the same statistical accuracy. The procedure is performed for the ABS injection modes $|1\rangle$ and $|1\rangle + |2\rangle$ to compare two different intensities (Fig. 6.1).

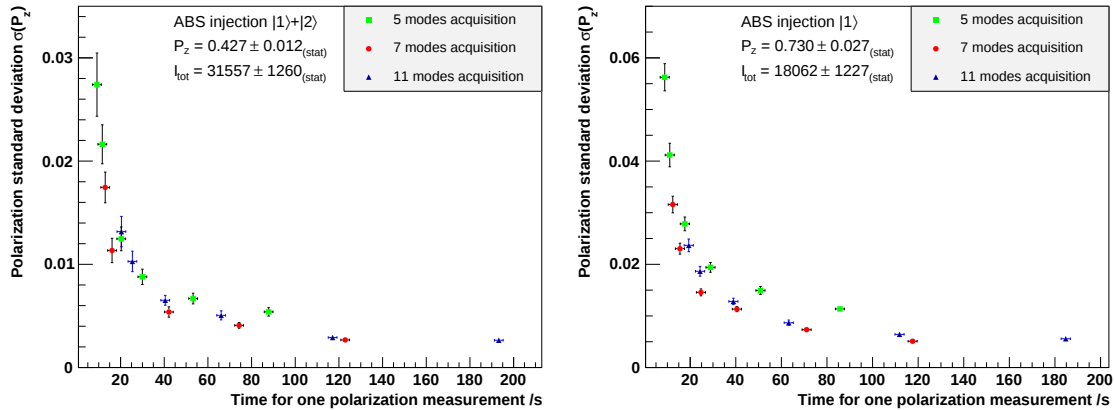


Fig. 6.1.: Standard deviation of a polarization measurement as function of the acquisition time. The statistical error of the polarization decreases with a longer measurement time. An error of ± 2 s is estimated for the acquisition time. This time uncertainty is the result of the irregular start of the time spectrum acquisition (delay time until the next chopper trigger). The histograms used to calculate the Gaussian fit are provided in Fig. C.7 (for the ABS state $|1\rangle$ injection). The plots in the panels on the left and right side are based on 2465 and 5560 measurements, respectively.

The statistical error decreases with increasing acquired time, a standard deviation of 0.01 requires about 60 seconds acquisition time with the intensity provided by the state $|1\rangle$ injection ($\sum_a I_a \approx 18000$). This acquisition time requires 11 modes at 10 chopper cycles or 7 modes at 20 chopper cycles, the chopper frequency is 2.2 Hz. The higher intensity of the ABS off mode reduces the error by one half and provides a standard deviation of about 0.005 after 60 seconds. The sequence with 5 modes has a systematically larger deviation from the average in both cases and is not used for typical measurements; however, a polarization could be measured in less than 10 seconds with this sequence.

6.1.3. Polarization Results

The atomic polarization has been measured for the three ABS injection modes. The measurement is performed with a sequence of 7 modes and 15 chopper cycles at 2.1 Hz; the magnetic holding field is set to $B = 0.74$ mT at the center of the storage cell. The distribution of the hyperfine state populations for each ABS injection mode is shown in Fig. 6.2 and the polarization results are listed in Eq. (6.2).

$$\begin{aligned}
 P_z(|1\rangle) &= 0.727 \pm 0.008_{\text{stat}} \pm 0.004_{\text{sys}} && \text{for the injection of state } |1\rangle \\
 P_z(|2\rangle) &= 0.073 \pm 0.006_{\text{stat}} \pm 0.002_{\text{sys}} && \text{for the injection of state } |2\rangle \\
 P_z(|1\rangle + |2\rangle) &= 0.421 \pm 0.005_{\text{stat}} \pm 0.003_{\text{sys}} && \text{for the injection of states } |1\rangle + |2\rangle.
 \end{aligned} \tag{6.2}$$

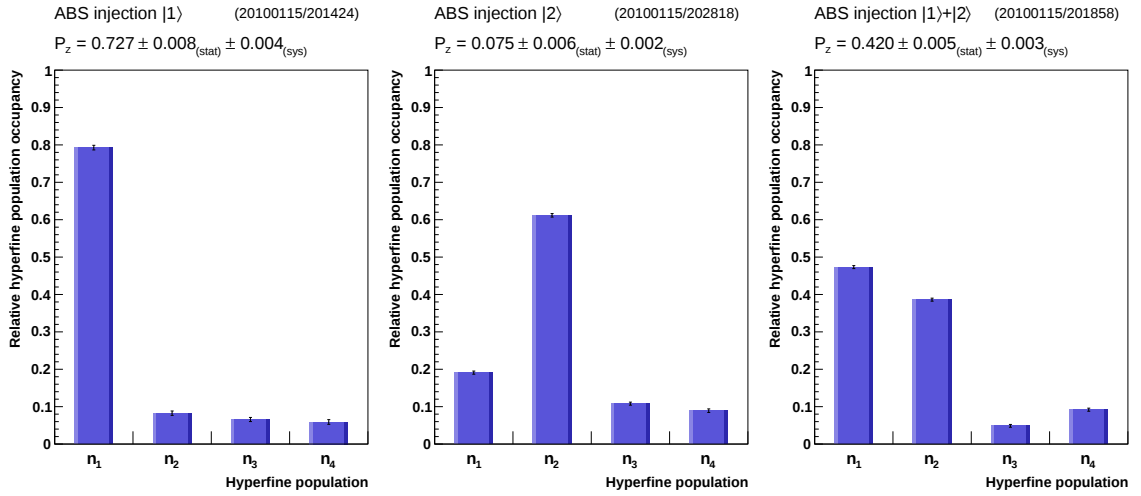


Fig. 6.2.: Polarization and relative hyperfine state population of hydrogen atoms of the beam sampled from the storage cell, generated with three ABS injection modes. The acquisition is performed with a sequence of 7 signals with each 15 chopper cycles at 2.1 Hz and a magnetic holding field of $B = 0.74$ mT. From left to right the injected states are $|1\rangle$, $|2\rangle$, and $|1\rangle + |2\rangle$ respectively. The numbers in parentheses (top right) uniquely identify the measurement with the date and time of the acquisition in format YYYYMMDD/hhmmss. The population n_a are the relative hyperfine state populations $n_a = \frac{N_a}{\sum_a N_a}$, with N_a the absolute hyperfine state population and a = number of hyperfine states.

The following observations can be made based on the hyperfine state populations of Fig. 6.2. The injection of a single state does result in a dominating population of the respective state and the injection of the states $|1\rangle + |2\rangle$ also results in a larger presence of those states. The other states, however, are also present and their population is different depending on the injection mode.

The exact injection composition is unknown because the two sub-transitions of the ABS MFT can not be exactly calibrated (see Sec. 5.2.2), also the sextupole system has different transmission probabilities depending on the state before and after the transition [95]. Nevertheless, the non-ideal occupancy of the hyperfine states probably does not only originate from the injection, but is rather the result of the depolarization mechanisms taking place inside the storage cell. For instance, when the ABS MFT unit is not active the ABS injects the states $|1\rangle + |2\rangle$ only and it could be assumed that the two relative hyperfine state populations n_1 and n_2 are equal. The population n_2 , however, is smaller than n_1 (Fig. 6.2, right panel).

Two effects are responsible for the depolarization (or mixing of the hyperfine state populations) inside the target cell: the spin relaxation in wall collisions and the spin-exchange collision between two atoms. Spin relaxation takes place when the atoms collide with the wall of the target cell; this

effect is influenced by the geometry and surface of the storage cell. Atoms in a specific state can change to any other state and therefore the spin relaxation affects the distribution of the hyperfine state populations [85, 71]. This effect is strongly related to the specific type of target cell (e.g., geometry, construction, wall material) and is present regardless of the injection mode.

During a spin-exchange collision two atoms can change their state as long as the total angular momentum of the colliding pair is conserved. A nuclear or electron spin can therefore only be transferred between pairs of atoms with the same total angular momentum $\sum_i m_F$. The possible pairs of hyperfine states between which a spin-exchange is possible are listed in Table 6.2 [85].

$\sum_i m_F^{(i)}$	Hydrogen hyperfine pairs $ ab\rangle \leftrightarrow cd\rangle$
2	$ 11\rangle$
1	$ 12\rangle 14\rangle$
0	$ 13\rangle 22\rangle 24\rangle 44\rangle$
-1	$ 32\rangle 34\rangle$
-2	$ 33\rangle$

Table 6.2.: Possible hyperfine state pairs where a spin-exchange during a collision is possible. A pair $|ab\rangle$ can change to a pair $|cd\rangle$.

The pairs $|11\rangle$ and $|33\rangle$ can not exchange a spin during a collision and can not depolarize by a spin-exchange collision. Therefore, the spin-exchange mechanism is fully suppressed in an atomic gas composed solely of state $|1\rangle$; the only possibility for atoms in state $|1\rangle$ to change their state is by spin relaxation in wall collisions. On the contrary, pairs of $|22\rangle$ states have multiple possibilities to change their state in a collision. The suppression of spin-exchange and the higher probabilities of the n_2 population to change its state could explain why the n_1 population for the state $|1\rangle$ injection is larger than the n_2 population in the state $|2\rangle$ injection (Fig. 6.2, left and center panels). The spin-exchange mechanism could also be the reason for the lower n_2 population compared to n_1 , when the ABS injects states $|1\rangle + |2\rangle$ into the storage cell (Fig. 6.2, right panel).

6.1.4. Discussion

All polarization measurements in this chapter represent a value of the *atomic* polarization of a sample extracted from the center of the storage cell. This value, however, does not represent the real target polarization seen by the beam, mainly for the following two reasons [128]:

- The gas in the storage cell is also composed of H_2 molecules. These molecules can originate from the rest gas, they can be injected by the ABS, and could also stem from the recombination on the surface of the cell. The fraction of atoms and molecules from the sample beam is measured with the Target Gas Analyzer (TGA). The nuclear polarization of H_2 molecules which recombined inside the storage cell depends on the surface, temperature, and magnetic holding field [132], and is specific to the storage cell.
- the spin relaxation and recombination on wall collisions lead to an inhomogeneous target polarization because the density and number of walls collisions is different towards the open ends of the cell.

The sampling nature of the polarization measurement with the BRP requires the application of sampling corrections to correlate the average of the target polarization along the cell axis to the polarization measured on the sample. An absolute calibration of the BRP together with the storage cell will be performed in the COSY ring by measuring the left-right $dp^\uparrow$ elastic scattering asymmetry²; at a beam energy for which the analyzing power A_y^P is known.

²Unpolarized d beam with a polarized $H^\uparrow$ gas target.

6.2. Applications

6.2.1. Effect of the Magnetic Holding Field

To avoid depolarization the polarized atoms require a magnetic holding field. The strength of the magnetic holding field influences the hyperfine state occupancy because the effects of the spin-exchange collision and spin relaxation on wall collisions change with the field strength [85, 71]. For typical polarization measurements the magnetic holding field is set to ≈ 0.74 mT (which corresponds to a current of 2 A for the holding field coils; a current of 2.7 A induces a magnetic field of 1 mT at the center of the cell (see Fig. C.5)). At this low field $B \ll B_C$ the polarization of the mixed states is negligible and the Eq. (2.51) can be simplified to $n_1 - n_3$.

To verify that this magnetic field is adequate to avoid any depolarization the polarization is measured with different current settings on the target chamber coils. Figure 6.3 shows the effect of the magnetic holding field on the polarization. The absence of a magnetic holding field induces a large depolarization of $\Delta P_z \approx 0.1$; however, a field of 0.2 mT is sufficient to keep the polarization at almost the maximal value. Higher magnetic fields up to 3 mT marginally improve the polarization by $\Delta P_z \approx 0.01$.

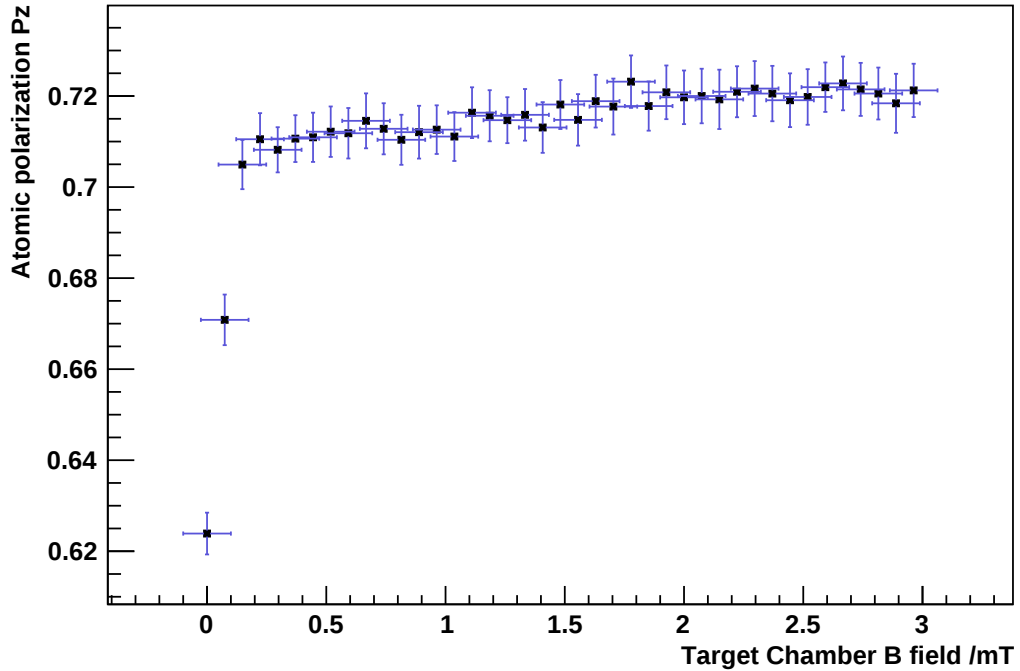


Fig. 6.3.: Effect of the magnetic holding field on the polarization $P_z = n_1 - n_3$. An error of $\Delta B = 0.1$ mT is given by the hall probe, the polarization error is calculated with the observed variation of multiple measurements for the same field, and also includes the systematic error.

The sharp drop of the polarization when the magnetic holding field is zero, raises the question of how the hyperfine state populations are modified due to the absence of a field. The hyperfine state populations have been measured with a zero field and are compared in Fig. 6.4 to the standard field used ($B = 0.74$ mT).

For the state $|1\rangle$ injection (Fig. 6.4, left) the reduced n_1 population due to the zero field is distributed in n_2 and n_3 and the polarization is reduced by $\delta P_z = -0.13$. For the state $|2\rangle$ injection (Fig. 6.4, center) the n_2 population loss is distributed into n_1 and n_3 and the polarization is reduced only by $\delta P_z = -0.02$. For the states $|1\rangle + |2\rangle$ injection (Fig. 6.4, right) the n_1 population loss is completely

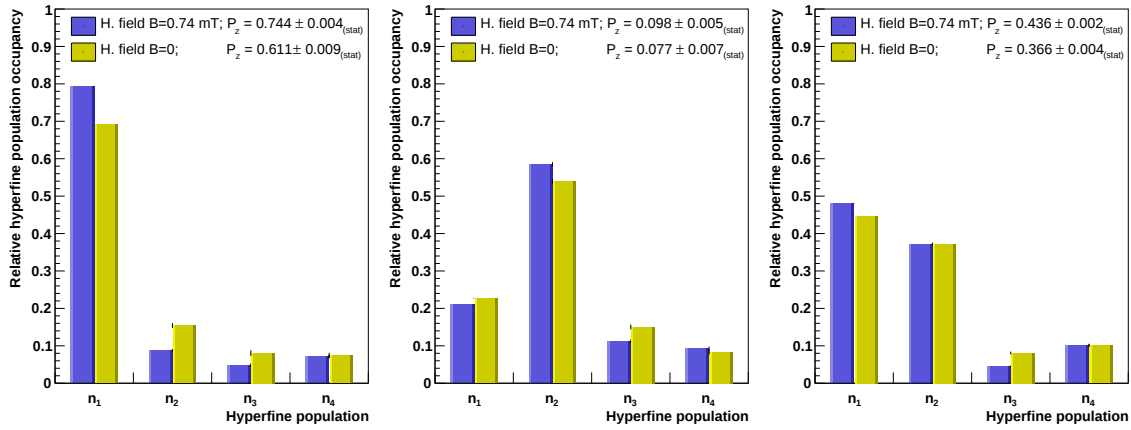


Fig. 6.4.: Polarization and relative hyperfine state occupancy of the three ABS injection modes with and without a magnetic holding field. The intensities are acquired with 7 modes, 20 chopper cycles with a frequency of 2.3 Hz. The error is less than 0.01 for all values.

transferred to n_3 which reduces the polarization by $\delta P_z = -0.07$. In all three injection cases the n_4 population is unaffected by the absence of a magnetic holding field within the error.

This effect of mixing the states $|1\rangle$, $|2\rangle$ and $|3\rangle$ but not $|4\rangle$ can be explained by the zero magnetic field. In the absence of magnetic holding field the atoms in the triplet $m_F = 1$ are all at the same energy level and can change the state within this triplet without energy exchange because the state is threefold degenerate (see Fig. 2.1). On the other hand, atoms in the singlet state $|4\rangle$ can not change their state without a photon exchange because they are separated from the other states by the hyperfine energy difference.

In addition to the effect of changing the hyperfine state occupancy, the magnetic field also influences the mixing of the states $|2\rangle$ and $|4\rangle$ and its strength enters in the calculation of the polarization (Sec. 2.3.1). The magnetic holding field will be operated around 1 mT for the PAX spin-filtering studies, then how relevant for the polarization is a field strength in the order of a mT? Using the relative hyperfine state populations of Fig. 6.2 the effect of different hypothetical holding fields are listed in Table 6.3.

Holding magnetic field /mT	$P_{z(1\rangle)}$	$P_{z(2\rangle)}$	$P_{z(1\rangle+ 2\rangle)}$
0	0.7270	0.0829	0.4245
0.74	0.7267	0.0753	0.4202
10	0.7225	-0.0183	0.3675
100	0.7061	-0.3832	0.1620

Table 6.3.: Polarization of hydrogen atoms based on the three measurements of the hyperfine state populations taken from Fig. 6.2 calculated with different hypothetical magnetic holding fields. The relative hyperfine populations were measured with a holding field of $B = 0.74$ mT. The systematic and statistical errors are unchanged from (6.2).

The small effect of the holding field for $P_{z(|1\rangle)}$ originates from the fact that the population n_2 and n_4 are almost equally large and their impact on the polarization cancels out (Fig. 6.2, left). In a strong field $B > 50.7$ mT the state $|2\rangle$ carries a negative polarization (see Fig. 2.1) and therefore reduces the polarization of $P_{z(|2\rangle)}$ and $P_{z(|1\rangle+|2\rangle)}$. The value for 100 mT in Table 6.3, however, can not be used to extrapolate the polarization measured at $B = 0.74$ mT because the hyperfine state occupancy will be different in a higher field and the polarization will probably increase in higher fields instead of being reduced (as in Tab. 6.3). This polarization increase in larger fields, due to reduced depolarization effects, can be seen already from the measurement in Fig. 6.3 at 3 mT.

6.2.2. Effect of the Cell Movement

A possibility to open the storage cell to accommodate the beam at injection energy is required for the measurements at AD (see Sec. 4.3). A prototype of an openable storage cell has been used for the calibration and polarization measurements. The two halves of the storage cell have to close tightly along the cell to maintain a high gas density. However, a possible overlap at the contact line might trap atoms and reduce the polarization because the atoms escaping back into the cell have lost their polarization due to spin relaxation on wall collisions. Due to the opening mechanism the storage cell geometry might be slightly different after every movement. This might lead to different polarization values. Also because the mechanics will have to be operated many times the polarization has to be stable between the opening cycles.

In Fig. 6.5 the polarization is measured after several opening and closing cycles. When the cell is open, the BRP signal is zero and the polarization can not be measured; when the cell is closed, the polarization is measured for 10-15 times. All polarization measurements belonging to a cycle are fitted to the indicated value. In all cases the polarization remains constant and is not affected by an opening cycle. The verification of the polarization stability was an important step to validate the new design of the opening mechanism. Additionally, the high polarization reached with this special design is an important improvement compared to previous designs [139]. Another important aspect to be tested in the future is the long term mechanical stability of the mechanism and the aging of the storage cells with hundreds of opening cycles to come.

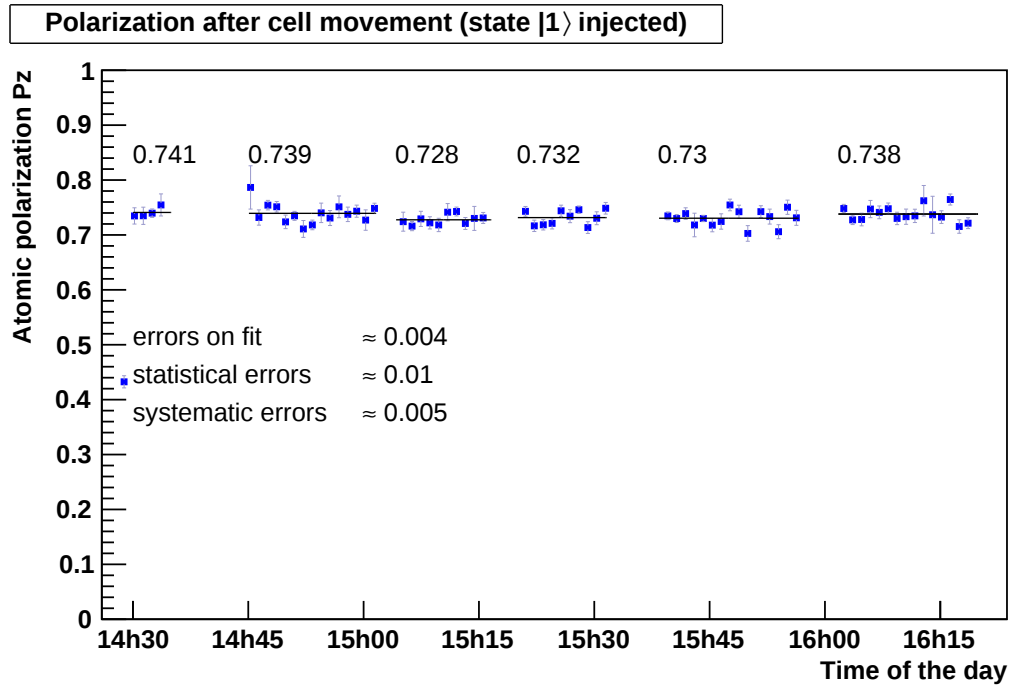


Fig. 6.5.: Polarization stability after several cell movements.

6.2.3. Polarization and ABS Intensity over a Nozzle Cycle

Another important experimental aspect of the polarized internal target is the span of time in between two nozzle regenerations (Sec. 4.2) and the stability of the polarization during this time. Figure 6.6 shows the polarization and total intensity over a full nozzle cycle which lasted 3.5 days. The polarization is stable during the full cycle and the intensity is steadily increasing until the icing eventually reduces and stops the atomic beam. The observed increase of the intensity might also

be due to an increase in the emission current. The signal is normalized to the emission current; however, during this measurement the emission current increased above 1 mA and went out of scale for the CAMAC ADC and was therefore not normalized. The bottom plot shows the last four hours of the cycle. The variation of the measured polarization increases at the end of the cycle when the intensity drops to a low level but the absolute value is not affected. Further tests will be performed to increase the cycle duration. One possibility is to reduce the cooling temperature of the discharge tube. A lower temperature (e.g., $-10\text{ }^{\circ}\text{C}$ instead of $15\text{ }^{\circ}\text{C}$) reduces the recombination and requires less oxygen admixture which would reduce the ice build-up.

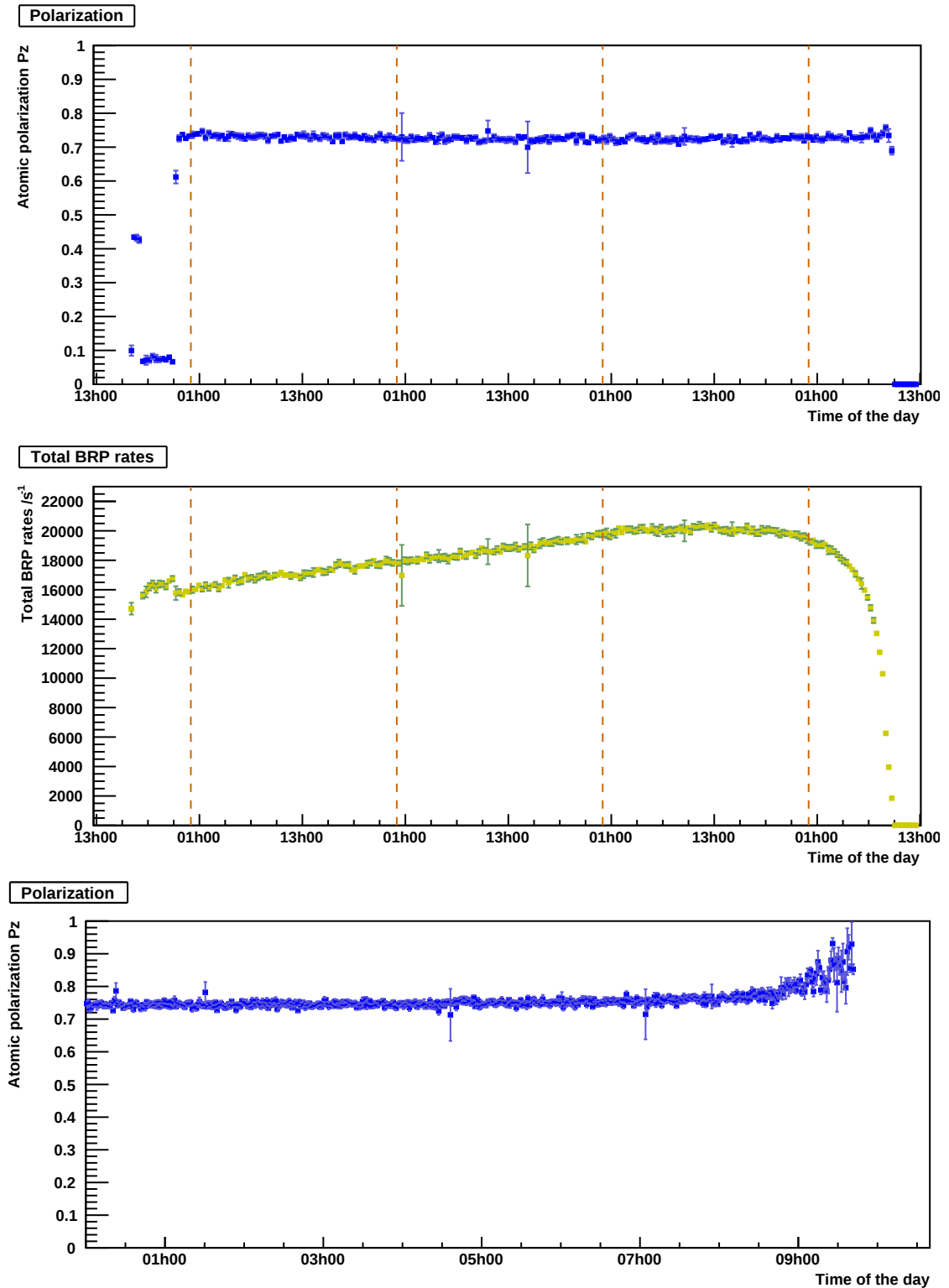


Fig. 6.6.: Polarization and ABS intensity during a nozzle cycle. The top two panels show the polarization and total intensity over a full nozzle cycle respectively. Vertical lines are placed at midnight. The fast drop in intensity due to icing of the nozzle at the end of the cycle is clearly visible. The dissociator was used at 1200 W power with an H₂ flow of 82 sccm and an O₂ flow of 0.09 sccm. The bottom panel shows the polarization of the last 4 hours before the interlock system deactivates the magnetron (20100103 is the date of the measurement). The polarization is stable regardless of intensity, only the statistical error increases when the intensity is reduced. For better readability in the two top panels, only every 200th data point is plotted.

7. CONCLUSION

The present work provides the theoretical and technical details necessary to operate and calibrate the Breit-Rabi polarimeter for the PAX spin-filtering experiments at COSY and AD. The theoretical foundation of the hyperfine splitting and hyperfine transitions as well as the theory of the calibration and polarization have been presented. A procedure has been developed and implemented to tune and calibrate the PAX Breit-Rabi polarimeter.

The numerical problem of the calibration has been solved with two nonlinear least square fit algorithms: the Gauss-Newton iteration and the Lagrange Multipliers algorithm. The inverse matrix operations use the Crout LU-decomposition algorithm with pivoting. Those algorithms and the accompanying linear algebra operators have been implemented in a C++ program and are used for the calibration and polarization analysis for hydrogen. The implementation of the deuterium analysis has been tested with simulated signals. The approach to use standard C++ without external numerical libraries or common math packages like MatlabTM required a larger upfront development effort but permitted to compile and to run the offline analysis software on Windows and integrate it in the online analysis within LabView. Without this portability, the development of the online polarization measurement would have been a major effort on LabView. Furthermore, the object oriented design of the program will enable an integration of the analysis in the central PAX program.

The slow control and acquisition program has been implemented with LabView. The design of the developed program is event based and separates the data acquisition from the control. This concept simplifies the addition of new functions which has been proven to be useful to develop dedicated measurements for this work. The functionalities necessary to operate the polarimeter, i.e., the magnetic field scan of the transitions, the polarization and the calibration measurements are operational for hydrogen. The calibration procedure also uses the integrated offline analysis program and is fully automatic. This automatization is important as the calibration procedure has to be repeated after any change in the configuration or after the installation in the ring.

The efficiencies measured with the calibration reached 100% for the SFTs, about 95% for the MFT 1-3 and about 85% for the MFT 2-3. The statistical errors are in the order of 1%. The low efficiency of the MFT 2-3 is unproblematic because the errors are small and the transition 2-3 is not required for a polarization measurement. The ratio σ_2/σ_1 of the sextupole transmission probabilities has been measured to be $\sigma_2/\sigma_1 = 0.9973 \pm 0.0005$.

Measurements of the polarization have been performed with the openable storage cell prototype. An atomic polarization of $P_z = 0.72$ is reached with the injection of the hyperfine state $|1\rangle$. The systematic error resulting from the calibration uncertainty is typically $\Delta P_z (\text{sys}) = 0.005$. The analysis of the statistical errors of the polarization has been discussed and showed that a standard deviation of $\Delta P_z (\text{stat}) = 0.01$ is reached with a measurement duration of 60 s. The effect of the holding magnetic field on the hyperfine state occupancy and on the polarization has been measured and discussed. Furthermore, it has been shown that the polarization is not affected by the opening cycles of the storage cell. This constitutes an important milestone because an openable storage cell design never before showed such a high polarization. In addition, it is a requirement for the planned operation at AD/CERN. The polarization is also stable over the time in between two nozzle regenerations and also during the various measurements performed for this work.

The stability of the chopper motor and trigger will be improved to avoid any shift in the time spectrum and eliminate wrong trigger events. The TGA analysis which was not part of this work

will have to be performed and merged with the polarization measurement procedure. Also the LabView data acquisition has to be merged with the central DAQ of the silicon detectors. The deuterium calibration will be performed for the installation at AD/CERN but is not required for the planned operation at COSY.

The Breit-Rabi polarimeter and the developed procedures for the calibration and the polarization measurement have been shown to function reliably during this work and are ready for the new assignment in the PAX spin-filtering studies. For the spin-filtering of antiprotons at AD the polarimeter will take an important part by providing the only calibration standard to interpret the $\bar{p}d^\uparrow$ scattering asymmetries.

Appendices

A. OPERATING PARAMETERS

The coils for the HFTs are fed by DC power supplies which are controlled by an input voltage from the slow control system. The power supply model with their output current and input voltages are listed in Table A.1. The ABS transition parameters are provided in Table A.2. For the BRP the SFT gradient is positive and the MFT gradient is negative. The MFT transitions are separated into two groups due to the cross-talk with the SFT magnetic field. When the SFT is operated alone, the MFT magnetic fields are set to a value between the mxxc14 and mxxc24 modes. A complete absence of the MFT magnetic field would lead to a situation where the SFT transition is outside its resonance. The BRP HFT parameters are listed in Table A.3.

Table A.1.: Power supplies used for the HFT coils.

HFT	Coil	Power supply	DAC rack/channel	Input control /V	Output current /A
ABS SFT	homogeneous	KEPCO bipolar	9/2	0 to ± 10	0 to ± 10
ABS SFT	gradient	Heinzinger LNG 32-3	9/3	0 to 10	0 to 3
ABS MFT	homogeneous	Heinzinger LNG 32-3	9/6	0 to 10	0 to 3
ABS MFT	gradient	KEPCO bipolar	9/7	0 to ± 10	0 to ± 3
BRP SFT	homogeneous	KEPCO bipolar	22/2	0 to ± 10	0 to ± 5
BRP SFT	gradient	Heinzinger LNG 32-3	22/3	0 to 10	0 to 3
BRP MFT	homogeneous	Heinzinger LNG 32-3	22/6	0 to 10	0 to 3
BRP MFT	gradient	KEPCO bipolar	22/7	0 to ± 10	0 to ± 2

Table A.2.: ABS injection modes and operating parameters for the MFT for hydrogen.

State injected	Transition mode	Transition name	Gradient direction	Frequency /MHz	Homogeneous B field /A	Gradient B field /A
$ 1\rangle + 2\rangle$	-	rfoff	-	0	0.6	0.9
$ 2\rangle$	MFT 1-3	m23m12	positive	66	0.48	1.5
$ 1\rangle$	MFT 2-3	m23	positive	66	0.45	0.75
$ 1\rangle$	MFT 2-3	m12m23	negative	66	0.62	-0.6

Table A.3.: Tuning parameters for the BRP transitions.

Transition active	Transition designation	SFT RF /MHz	SFT B Hom /A	SFT B Grad /A	MFT RF /MHz	MFT B Hom /A	MFT B Grad /A
BRP off	rfoff	0	1	0.36	0	0.39	1.2
SFT 1-4	s14	1446.9	0.4	0.36	0	0.39	1.2
SFT 2-4	s24	1446.9	1.61	0.36	0	0.39	1.2
MFT 1-3	m13c14	0	0.4	0.36	65	0.35	1.2
MFT 2-3	m23c14	0	0.4	0.36	65	0.27	1.2
MFT 1-3	m13c24	0	1.61	0.36	65	0.44	1.2
MFT 2-3	m23c24	0	1.61	0.36	65	0.34	1.2

B. DEUTERIUM SIGNAL MODES AND EFFICIENCIES

All possible BRP signals for deuterium are listed in Table B.1. The calibration efficiencies are listed in Table B.3. The possible ABS injection states for deuterium are listed in Table B.2.

Table B.1.: BRP signals for deuterium. 28 modes + off.

BRP mode	signal name	SFT-RF	SFT-B	MFT-RF	MFT-B
OFF	off	OFF	OFF	OFF	OFF
SFT 1-6	s16	ON	1-6	OFF	OFF
SFT 2-6	s26	ON	2-6	OFF	OFF
SFT 2-5/3-6	s25	ON	2-5	OFF	OFF
SFT 3-5	s35	ON	3-5	OFF	OFF
MFT 1-4	m14c16	OFF	1-6	ON	1-4
MFT 2-4	m24c16	OFF	1-6	ON	2-4
MFT 3-4	m34c16	OFF	1-6	ON	3-4
MFT 1-4	m14c26	OFF	2-6	ON	1-4
MFT 2-4	m24c26	OFF	2-6	ON	2-4
MFT 3-4	m34c26	OFF	2-6	ON	3-4
MFT 1-4	m14c25	OFF	2-5	ON	1-4
MFT 2-4	m24c25	OFF	2-5	ON	2-4
MFT 3-4	m34c25	OFF	2-5	ON	3-4
MFT 1-4	m14c35	OFF	3-5	ON	1-4
MFT 2-4	m24c35	OFF	3-5	ON	2-4
MFT 3-4	m34c35	OFF	3-5	ON	3-4
SFT 1-6 + MFT 1-4	m14s16	ON	1-6	ON	1-4
SFT 1-6 + MFT 2-4	m24s16	ON	1-6	ON	2-4
SFT 1-6 + MFT 3-4	m34s16	ON	1-6	ON	3-4
SFT 2-6 + MFT 1-4	m14s26	ON	2-6	ON	1-4
SFT 2-6 + MFT 2-4	m24s26	ON	2-6	ON	2-4
SFT 2-6 + MFT 3-4	m34s26	ON	2-6	ON	3-4
SFT 2-5 + MFT 1-4	m14s25	ON	2-5	ON	1-4
SFT 2-5 + MFT 2-4	m24s25	ON	2-5	ON	2-4
SFT 2-5 + MFT 3-4	m34s25	ON	2-5	ON	3-4
SFT 3-5 + MFT 1-4	m14s35	ON	3-5	ON	1-4
SFT 3-5 + MFT 2-4	m24s35	ON	3-5	ON	2-4
SFT 3-5 + MFT 3-4	m34s35	ON	3-5	ON	3-4

Injected states	ABS SFT	ABS MFT
$ 1\rangle, 2\rangle, 3\rangle$	OFF	OFF
$ 1\rangle, 2\rangle$	OFF or s35	m34
$ 1\rangle, 3\rangle$	OFF or s35	m34m23
$ 2\rangle, 3\rangle$	OFF or s35	m34m23m12
$ 1\rangle$	s26	m34
$ 1\rangle$	s26	m34m23
$ 2\rangle$	s26	m34m23m12
$ 1\rangle, 2\rangle$	s35	OFF
$ 1\rangle, 3\rangle$	s26	OFF

Table B.2.: ABS possible injection modes for deuterium with the MFT and SFT. The SFT is placed before the MFT and both gradients are positive.

Table B.3.: BRP calibration efficiencies for deuterium. 40 efficiencies + sextupole transmission probabilities.

Efficiency	SFT-B	MFT-B	Ideal	Efficiency	SFT-B	MFT-B	Ideal
ϵ_{s16}	1-6	OFF	1				
ϵ_{s26}	2-6	OFF	1				
ϵ_{s25}	2-5	OFF	1				
ϵ_{s36}	3-6	OFF	1				
ϵ_{s35}	3-5	OFF	1				
$\epsilon_{m14r12c16}$	1-6	1-4	1	$\epsilon_{m14r12c25}$	2-5	1-4	1
$\epsilon_{m14r23c16}$	1-6	1-4	1	$\epsilon_{m14r23c25}$	2-5	1-4	1
$\epsilon_{m14r34c16}$	1-6	1-4	1	$\epsilon_{m14r34c25}$	2-5	1-4	1
$\epsilon_{m24r12c16}$	1-6	2-4	0	$\epsilon_{m24r12c25}$	2-5	2-4	0
$\epsilon_{m24r23c16}$	1-6	2-4	1	$\epsilon_{m24r23c25}$	2-5	2-4	1
$\epsilon_{m24r34c16}$	1-6	2-4	1	$\epsilon_{m24r34c25}$	2-5	2-4	1
$\epsilon_{m34r12c16}$	1-6	3-4	0	$\epsilon_{m34r12c25}$	2-5	3-4	0
$\epsilon_{m34r23c16}$	1-6	3-4	0	$\epsilon_{m34r23c25}$	2-5	3-4	0
$\epsilon_{m34r34c16}$	1-6	3-4	1	$\epsilon_{m34r34c25}$	2-5	3-4	1
$\epsilon_{m14r12c26}$	2-6	1-4	1	$\epsilon_{m14r12c35}$	3-5	1-4	1
$\epsilon_{m14r23c26}$	2-6	1-4	1	$\epsilon_{m14r23c35}$	3-5	1-4	1
$\epsilon_{m14r34c26}$	2-6	1-4	1	$\epsilon_{m14r34c35}$	3-5	1-4	1
$\epsilon_{m24r12c26}$	2-6	2-4	0	$\epsilon_{m24r12c35}$	3-5	2-4	0
$\epsilon_{m24r23c26}$	2-6	2-4	1	$\epsilon_{m24r23c35}$	3-5	2-4	1
$\epsilon_{m24r34c26}$	2-6	2-4	1	$\epsilon_{m24r34c35}$	3-5	2-4	1
$\epsilon_{m34r12c26}$	2-6	3-4	0	$\epsilon_{m34r12c35}$	3-5	3-4	0
$\epsilon_{m34r23c26}$	2-6	3-4	0	$\epsilon_{m34r23c35}$	3-5	3-4	0
$\epsilon_{m34r34c26}$	2-6	3-4	1	$\epsilon_{m34r34c35}$	3-5	3-4	1
σ_2/σ_1			1				
σ_3/σ_1			1				

C. ADDITIONAL PLOTS

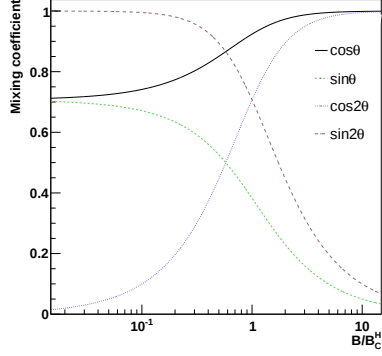


Fig. C.1.: Mixing coefficient functions for hydrogen versus the external magnetic field normalized to the critical field calculated with Table 2.1. The coefficients are used to calculate the polarization contribution of each hyperfine state for hydrogen and result in the plot 2.2 using Eq. (2.51).

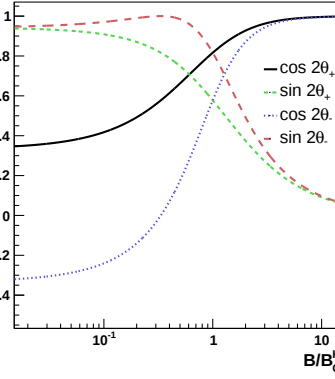
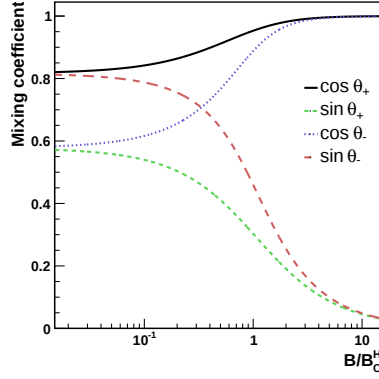


Fig. C.2.: Mixing coefficient for deuterium versus the external magnetic field normalized to the critical field. The functions on the left plot are used to calculate the functions on the right plot. The coefficients are used to calculate the Polarization contribution of each hyperfine state for deuterium and result in Fig. 2.3 using Eq. (2.55) and (2.58).

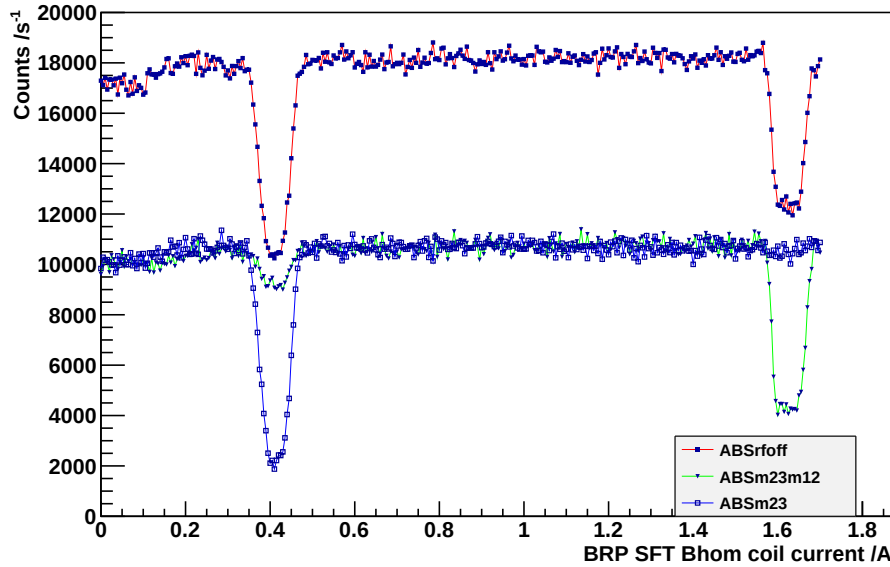


Fig. C.3.: BRP SFT scan with different ABS injection states. This plot is used to verify the injection quality. The scan ABSm23m12 is performed with the ABS injection of state $|2\rangle$, in this case the SFT 1-4 transition should not be visible if the storage cell does not contain any atoms in state $|1\rangle$. However, the SFT 1-4 (on the left) reduces the ABSm23m12 signal meaning that the storage cell contains a non zero N_1 population. The ABSm23 scan, however, is barely affected by the SFT 2-4 transition; the N_2 population is very low when the ABS injects the state $|1\rangle$.

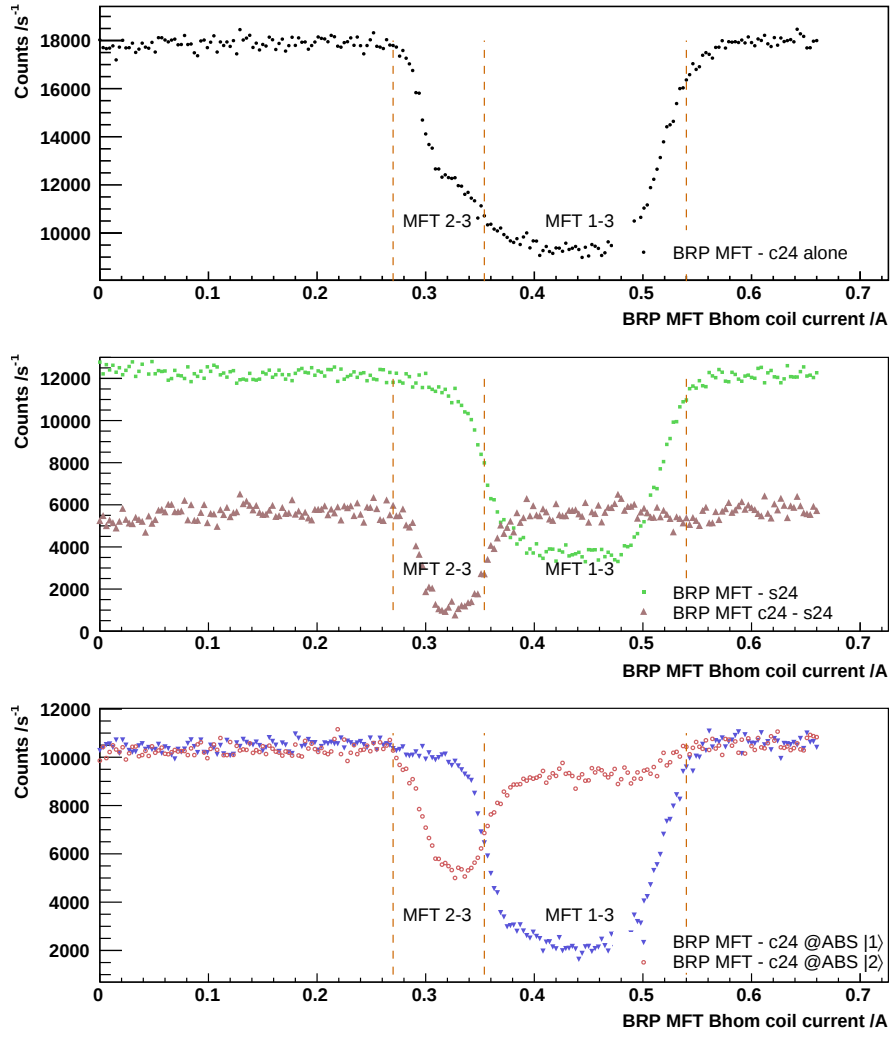


Fig. C.4.: Scan of the homogeneous magnetic field of the BRP MFT with the c24 magnetic field setting. The central plot uses the SFT 2-4 to reveal the MFT 1-3 region. The bottom plot uses the two ABS MFT injection modes to separate the MFT 2-3 and MFT 1-3 regions.

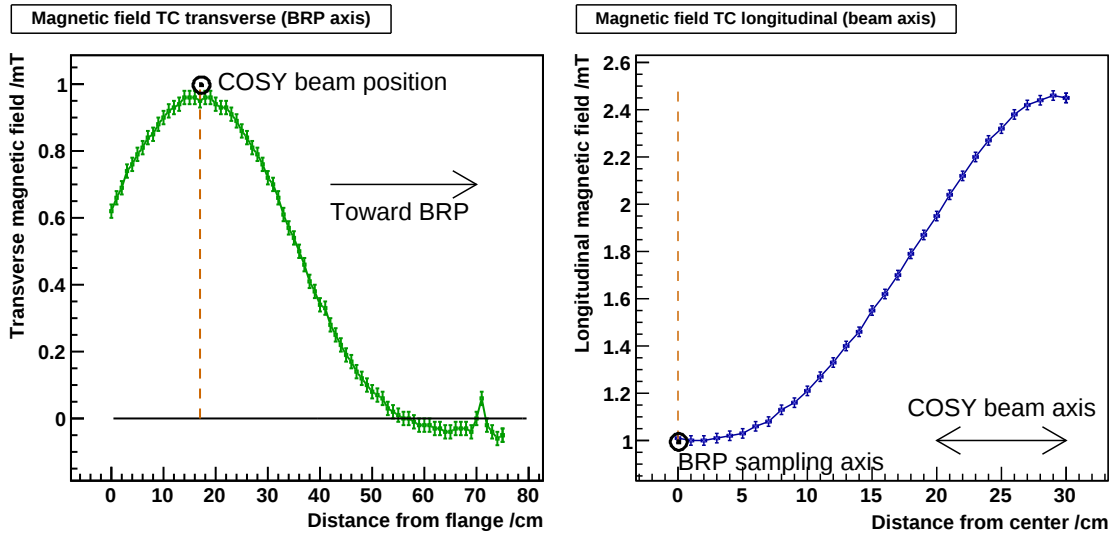


Fig. C.5.: Magnetic field scan of the target chamber with a coil current of 2.7 A.

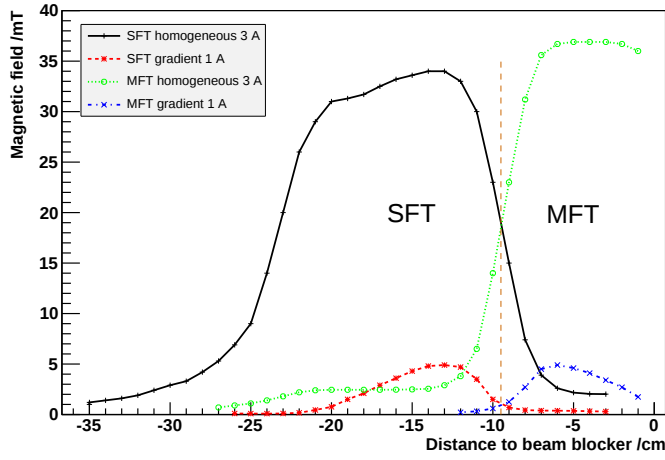


Fig. C.6.: Magnetic field scan of the BRP transitions.

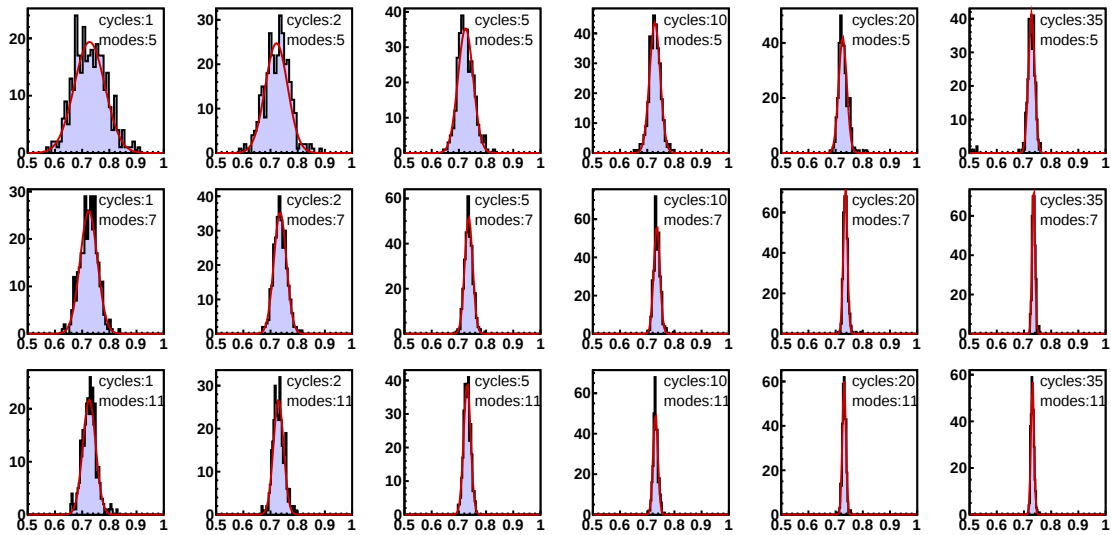


Fig. C.7.: Histograms used for the error analysis of Fig. 6.1. The polarization of each combination of chopper cycle and run sequence is stored in a histogram. The fitted Gaussian provides the standard deviation of the polarization measurement of this specific combination. The scale range is identical for all histograms, but the binning is adapted to the width to optimize the accuracy of the fit.

D. COMPRESSION TUBE CALIBRATION

The absolute intensity of the ABS is measured with a compression tube in the analyzing chamber. This method is used to check and optimize the performance of the ABS. The compression tube is placed on the beam axis at the focusing point of the sextupole magnets in the center of the target chamber where the target cell is later located for the experiment. The flow of the ABS beam and thus its intensity is directly proportional to the pressure in the compression tube. However, the correlation between the flow and the pressure in the compression tube is unknown and has to be measured. The calibration is achieved by using the pressure decay of a known volume V_{cal} through a needle valve into the vacuum of the compression tube. A baratron gauge measures the pressure in the calibrated volume and an ion gauge measures the pressure in the compression tube. The setup is shown in Fig. D.1.

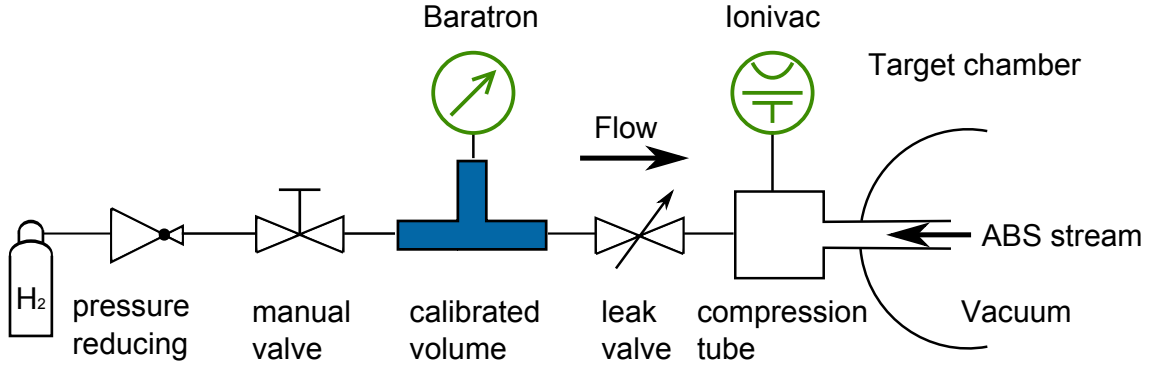


Fig. D.1.: Schematic view of the compression tube calibration setup. The baratron gauge measures the pressure in the calibrated volume V_{cal} . When the needle valve is open the ion gauge in the compression tube measures the pressure increase caused by the gas flow streaming from the calibrated volume. The ABS is turned off during the calibration. Once calibrated, the compression tube pressure p_{CT} provides a direct measurement of the ABS beam intensity (indicated by the ABS stream arrow).

The gas flow Q escaping from a known volume V_{cal} is defined by the pressure change over time with

$$Q = \frac{dp_{cal}(t)}{dt} V_{cal}. \quad (D.1)$$

The exponential pressure decay over time caused by the escaping gas flow is then described by the decay constant a :

$$p_{cal} = p_{cal}^0 \cdot e^{-at}$$

with $p_{cal}^0 = p_{cal}(t = 0)$ the initial pressure in the calibrated volume. The decay graphs measured for a starting pressure of about 100 mbar for both gauges is plotted in the top figures D.2. With Eq. (D.1) the gas flow is then expressed as

$$Q = ap_{cal}V_{cal}. \quad (D.2)$$

The flow Q escaping the calibrated volume and defined by the Eq. (D.2) passes through the compression tube into the vacuum of the target chamber. The pressure increase in the compression tube resulting from the flow is measured by the ion gauge. Since both the baratron and ion gauge measure the pressure decay simultaneously, a direct correlation between the flow Q and

the compression tube pressure p_{CT} is achieved. For every pressure p_{cal} in the calibrated volume corresponds a compression tube pressure p_{CT} and a flow Q from (D.2). This calibration of the compression tube pressure p_{CT} and gas flow $Q(p_{CT})$ is plotted in the bottom panel in Fig. D.2. The flow is converted in molecules per seconds using the standard ideal gas law $PV = NkT$. The molecular flow is calculated with

$$Q(p_{CT}) = \frac{ap_{cal}V_{cal}}{10kT} \frac{H_2}{s}. \quad (D.3)$$

The factor 10 above results from the conversion of mbar·liter to Pa·m⁻³. The linear dependency of the compression tube pressure and the gas flow is fitted with the function

$$Q(p_{CT}) = b + c \cdot p_{CT} \frac{H_2}{s}. \quad (D.4)$$

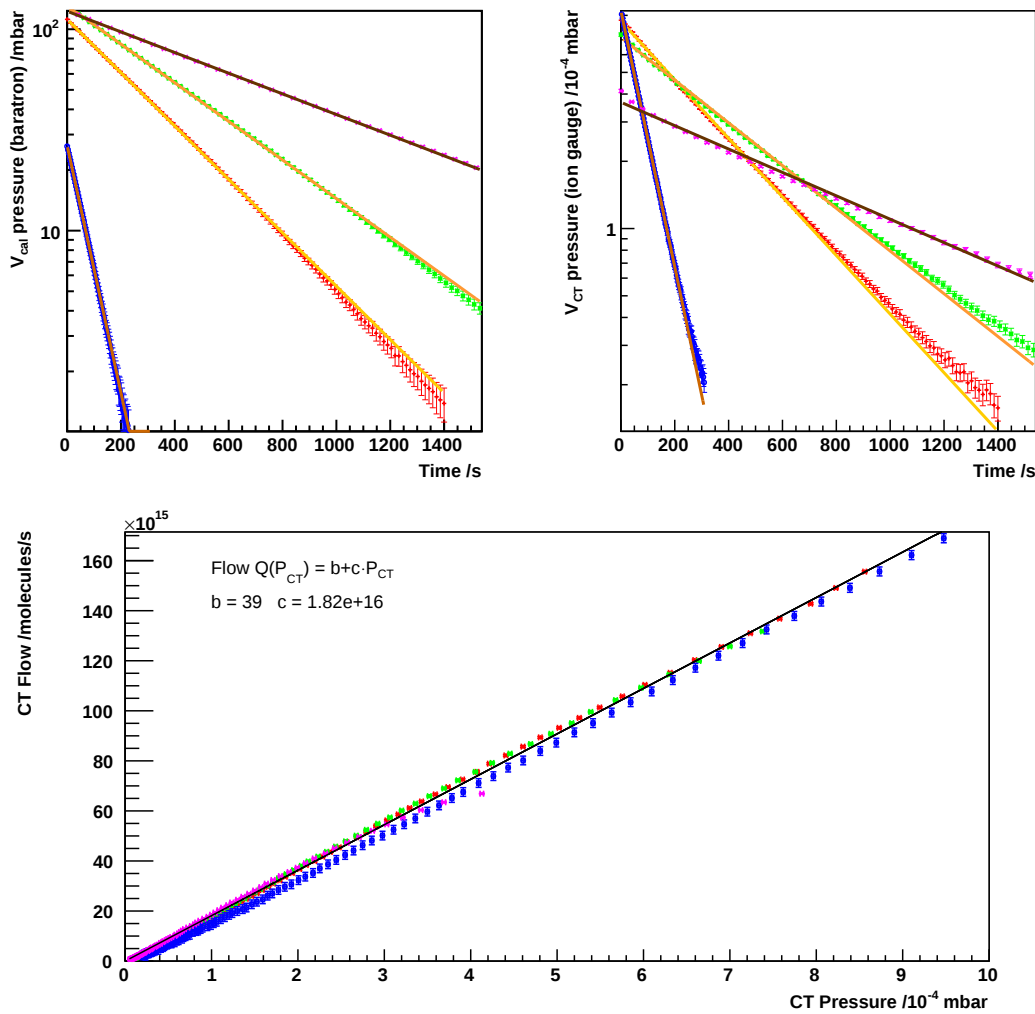


Fig. D.2.: Top left and right: pressure decay of the baratron and ion gauge sensors with fitted exponential function. Multiple measurements were done with different flows. The steeper line corresponds to a larger flow, e.g., a greater opening of the needle valve. The flatter line corresponds to a smaller flow. Bottom: calibration of the flow Q versus the compression tube pressure p_{CT} measured by the ion gauge. For better readability only 10% of the points are shown in the plots; however, the fits are done with the full data set. The ABS intensity is directly proportional to the compression tube pressure p_{CT} .

The results of the fitted calibration function (D.4) and measurement parameters are shown in Table D.1. The errors are calculated with error propagation using a 10 mV ($\approx 10^{-7}$ mbar) error for the

gauge reading on the ADC. Equation (D.4) is used to calculate the intensity of the ABS for a given compression tube pressure. As visible in the bottom panel of Fig. D.2, the dependency of the flow against the pressure is linear for all measured flows. The slope of the line in the bottom panel of Fig. D.2 represents the conductance of the compression tube. Furthermore, larger or smaller calibration flows from the different measurements (shown in the top panels of Fig. D.2) do not affect the calibration results.

Table D.1.: Compression tube calibration results and parameters.

Parameter	Measured value or constant
Fit parameter b	$0 \pm 2.6 \times 10^7 \text{ (H}_2\text{/s)}$
Fit parameter c	$1.8158 \times 10^{16} \pm 5 \times 10^{12} \text{ (H}_2\text{/10}^{-4}\text{ mbar} \cdot \text{s)}$
Calibrated volume V_{cal}	18,87 ml
Baratron range	0-100 Torr $\rightarrow$ 0-10 Volt (linear)
Ion gauge range	$(0-10) \times 10^{-4} \text{ mbar} \rightarrow$ 0-10 Volt (linear)
Gauge estimated error	$\pm 10 \text{ mVolt} \simeq 10^{-7} \text{ mbar}$
1 Torr =	133.322368 Pa
k = Boltzmann constant	$1.38066 \times 10^{-23} \text{ J/K}$

Fig. D.3 shows the resulting intensity dependency of the ABS.

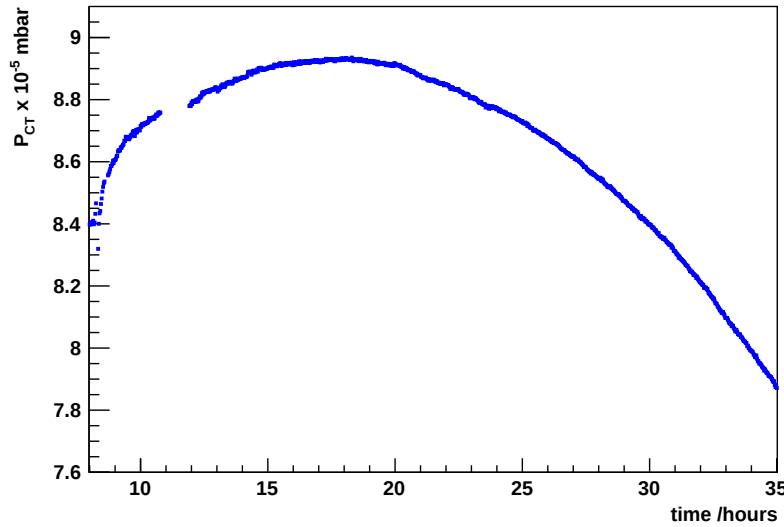


Fig. D.3.: As explained in Sec. 4.2 the ice formation on the nozzle surface improves the intensity at first but reduces the throughput over time by clogging the nozzle. The icing effect leads to a bell shaped intensity curve and the intensity drops quickly at the end of the cycle.

E. QUADRUPOLE MASS ANALYZER

E.1. QMA Optics and Voltages

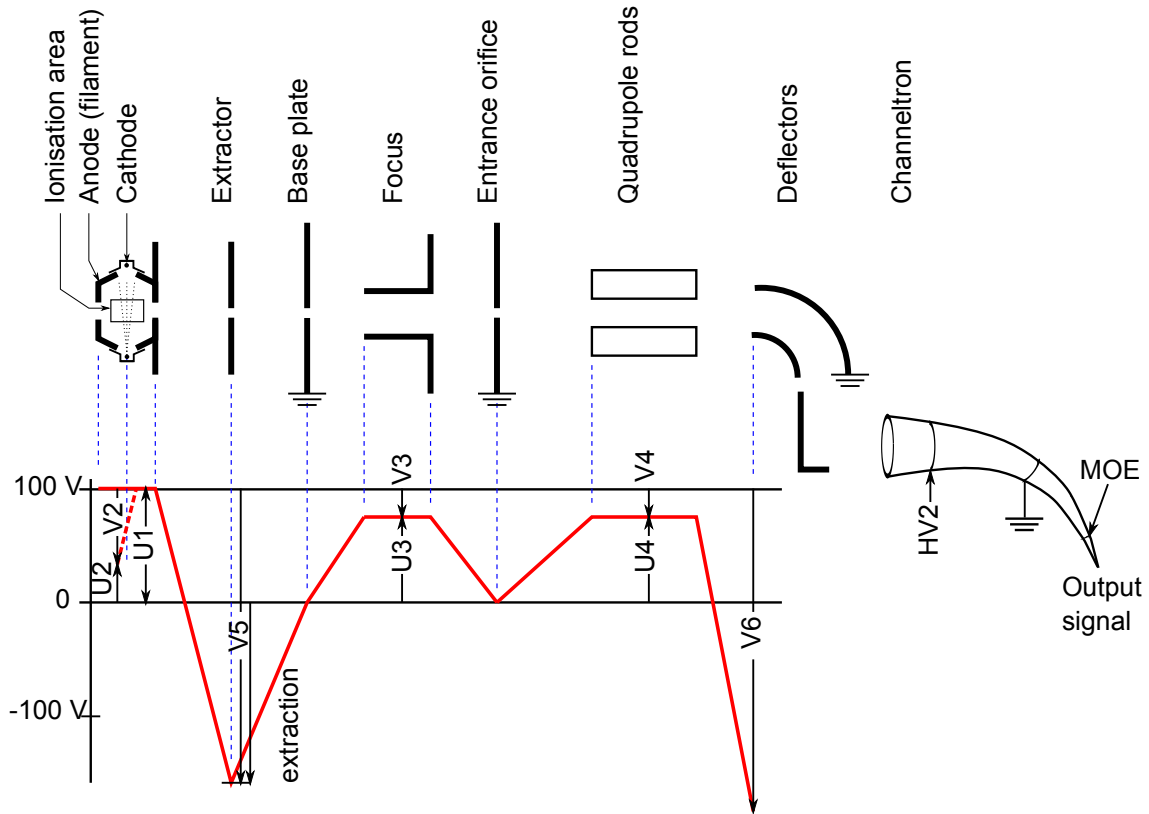


Fig. E.1.: QMA optics scheme. The QMA400 manual defines the V_i voltages [135], the setup for PAX BRP uses the U_i voltages. The MOE is grounded.

Table E.1.: QMA operating voltages for the TGA and BRP as used during this work.

QMA	U_1 /V	U_2 /V	U_3 /V	U_4 /V	U_5 /V	Extraction /V	HV1 /V	HV2 /V
TGA	90	20	77	81	-143	-162	69	2200
BRP	90	20	78	82	-148	-160	94	1850

E.2. Channeltron and Mass Scan

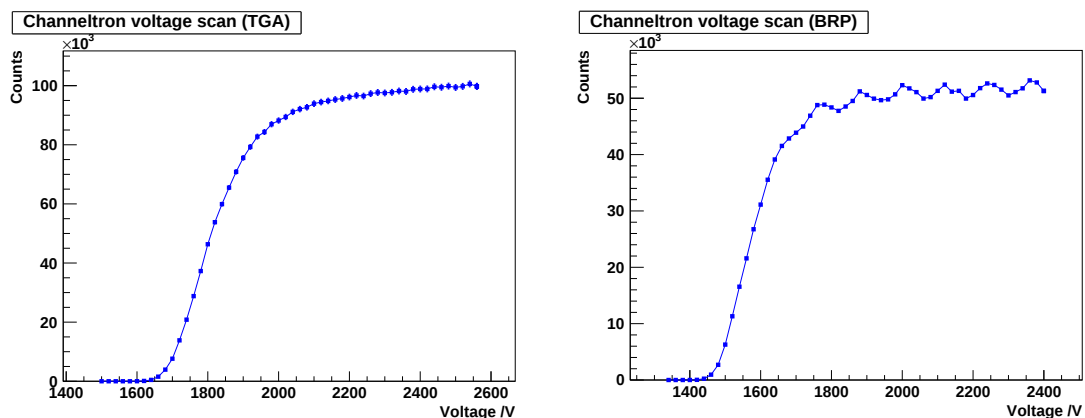


Fig. E.2.: Channeltron scan for the TGA and BRP. The best operating voltage is at the beginning of the plateau.

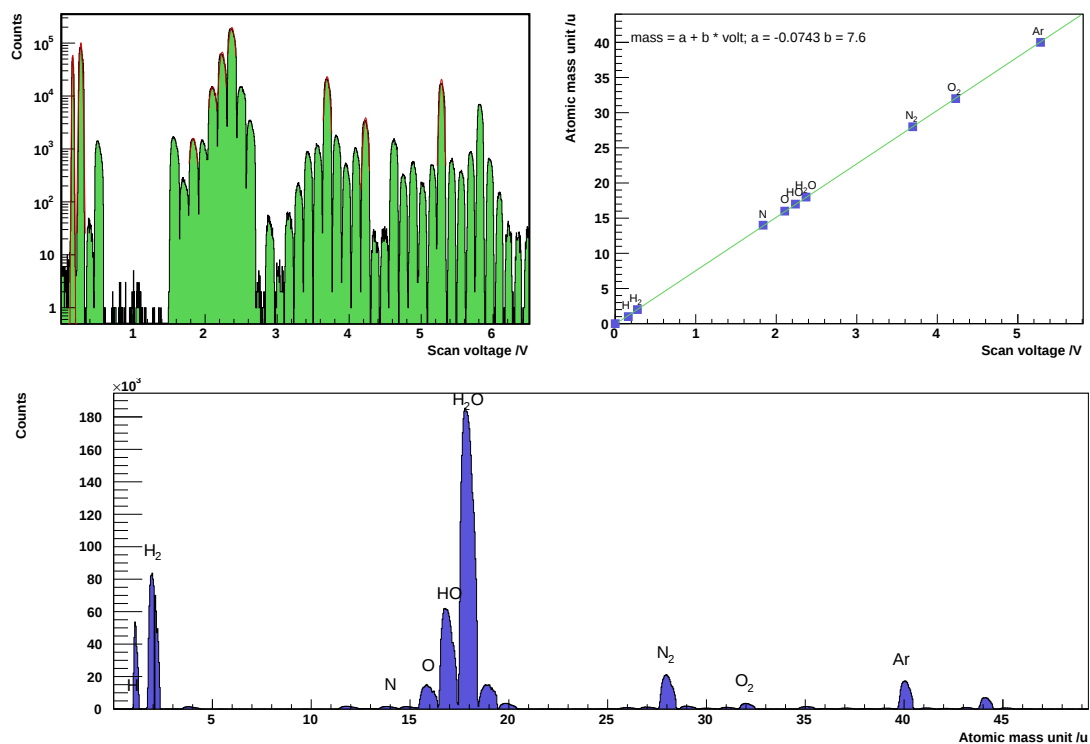


Fig. E.3.: Mass scan and calibration of the BRP QMA control voltage. Argon was fed into the chamber and used as reference for mass 40. Known mass peaks are fitted with a Gaussian and compared to the control voltage. The top right panel shows a perfect linearity between the control voltage and the atomic mass.

E.3. QMA Pictures

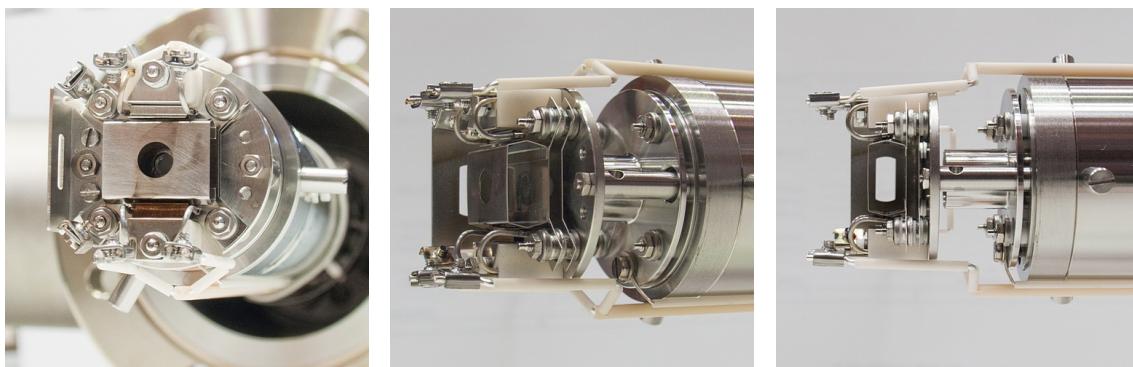


Fig. E.4.: Cross beam ionizer optics of the TGA QMA (identical to the BRP) taken at different angles. The entry baffle is seen on the left side of the ionization volume. The tube between the ionization volume and the housing of the quadrupoles is the focus optic.



Fig. E.5.: TGA chamber with QMA and chopper. The chopper baffle and beam blocker are seen on the right. The housing of the titanium sublimation pump is seen in the back.

F. SLOW CONTROL AND DATA ACQUISITION SOFTWARE

The slow control and data acquisition system are integrated into a Labview program (Sec. 4.7). The program is event driven and has two separated loops running in parallel, one for the control and logic and one for the acquisition. The advantage of the event-based approach instead of a sequential operation is that the acquisition is separated from the control and could also be hosted on a different computer. The control logic of different routines are programmed within their own event structure and the implemented sequences are independent of each other. For example, a magnetic field scan has a very different sequence compared to the calibration routine, but they both use the same acquisition logic and are not bound inside a global frame sequence. Additionally, the hardware control is idle during the acquisition but it is still responsive to user inputs. It is possible to change any hardware or sequence parameter during the running acquisition (e.g., open or close the beam shutter, tune a frequency, change the holding magnetic field). Figure F.1 shows a diagram of the general architecture concept with the control and acquisition loops connected by events. Both control and acquisition routines are either interacting in a sequential logic or can be controlled by the graphical user interface with the buttons and input controls. An automatic control sequence like a magnetic field scan or calibration procedure mimic a virtual operator by pushing the buttons or entering values in the input fields. This approach provides a constant overview of the hardware parameters and also permits to visualize (or intervene in) the running sequence. A screenshot of the graphical user interface is shown in Fig. F.2

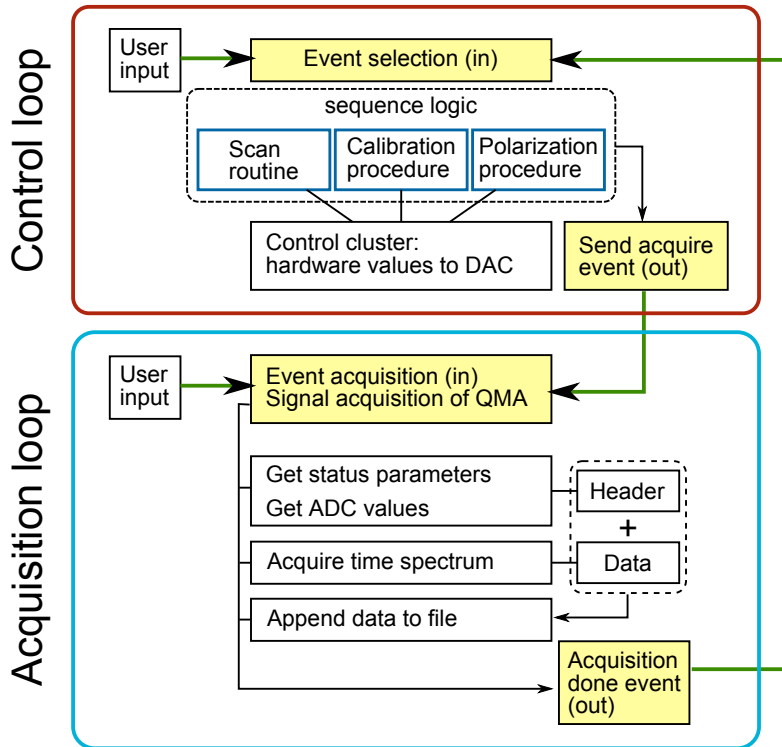


Fig. F.1.: Design of the Labview program. The control and acquisition loop are separated and call each other via events. The machine parameters set by the control loop are accessed by the acquisition routine with local variables. Each sequence logic (e.g., scan, polarization measurement) is implemented in its own event frame. The general sequential logic can be easily extended by adding a new event structure.

The control of the CAMAC DAC is a direct representation of the voltages used to control the HFT units. A specific mode for the ABS or BRP is set with the `Configuration_ABS(_BRP)` drop

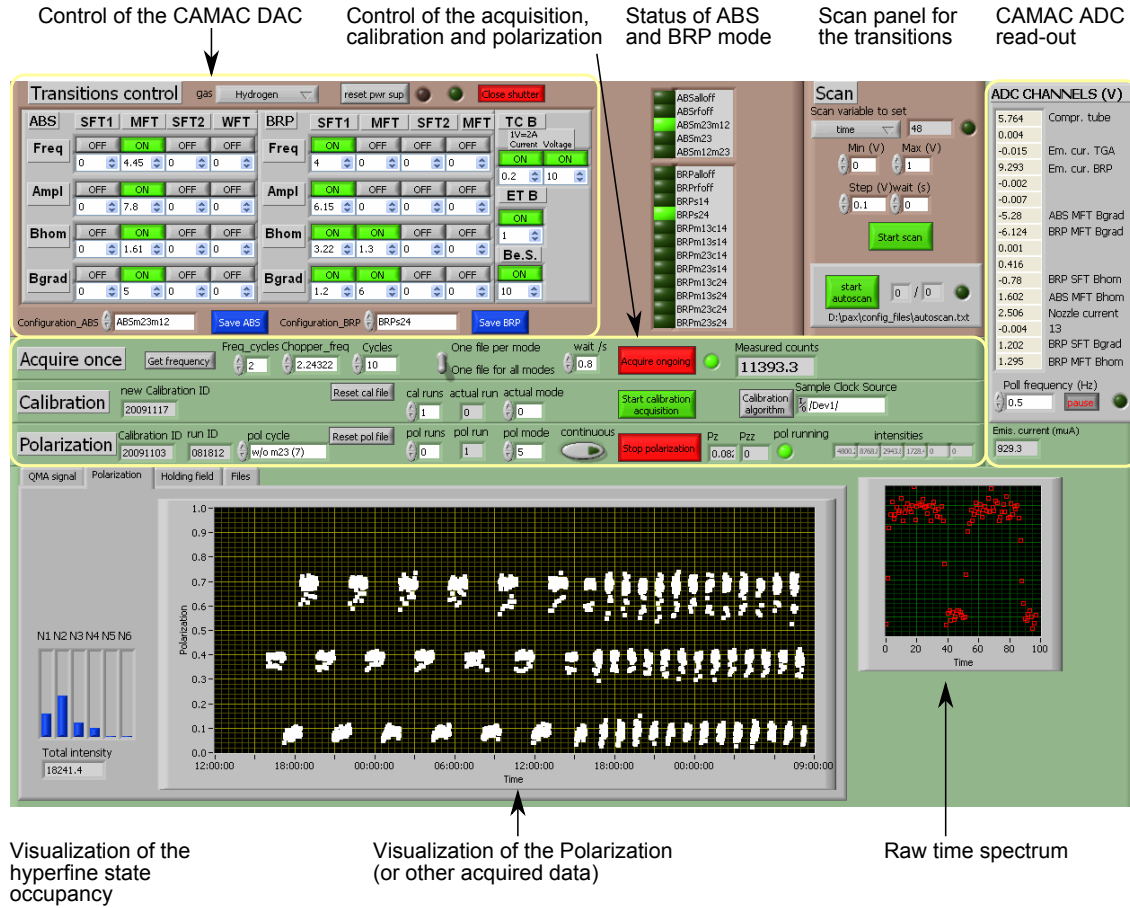


Fig. F.2.: Screenshot of the slow control software.

down selection; the parameters of the mode are loaded from a file. The actual status is indicated with a LED on the right. The control panel of the acquisition, calibration and polarization (center panel marked with an arrow) is used to set the acquisition parameters and start a polarization or calibration sequence.

The calibration procedure is performed as follows. The desired number of calibration cycles (typically 35) is specified in the input “cal_runs”, the number of chopper cycles for one acquisition (typically 10) is set in the input “cycles”. The button “Start calibration acquisition” starts the automatic sequence. The actual calibration cycle is indicated in the “actual_run” field and the actual calibration mode (1-33 for hydrogen) is indicated in the “actual_mode” field. When the calibration acquisition is terminated the analysis is started with the button “Calibration algorithm”. The results are displayed and a dialog presents the option to use or discard this calibration. If the calibration is accepted it is automatically used for the next polarization measurements.

The polarization measurement is started with the “Start polarization button”. The run sequence is selected in the drop down menu “pol_cycle”. The measurement will run continuously if the button “continuous” is pressed.

G. DATA ANALYSIS SOFTWARE

G.1. Program Design

The offline data analysis software is implemented in C++ and is compiled with GNU/g++ 4.4 on Linux and Windows. Only functionalities from the standard C++ library have been used to ensure the full portability to other compilers and operating systems. The program is called brprun and it is used to read and process the raw data generated by the data acquisition system and to solve the numerical problems for the polarization and the calibration. The general design is shown in Fig. G.1.

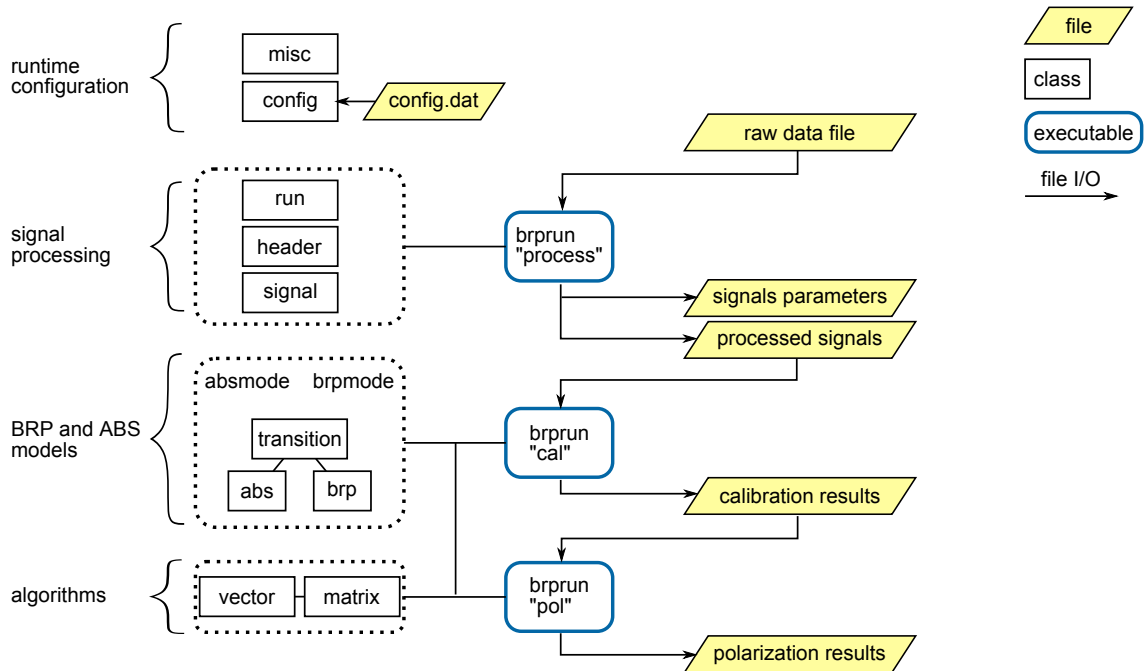


Fig. G.1.: Design of the signal processing and analysis software used for the offline and online analysis of the calibration and polarization measurements.

The components of the software are arranged in four categories: the runtime configuration, the signal processing, the mathematical model of the ABS and BRP and the generic algorithms. The runtime configuration is implemented in the `config` class and permits to change variables which should not be hard coded. The class reads the variables from the file “`config.dat`” and makes them available to all other components of the program. Typical runtime values are the correction factors discussed in Sec. 5.3, the chopper boundaries of the time spectrum, the error of the emission current etc.

The purpose of the signal processing components is to read the raw data generated by the DAQ and provide the condensed information needed by the calibration and polarization routines. The raw data is read by the `signal` class which uses the `header` class to parse the headers inserted before each time spectrum. All signals belonging to a polarization run are stored in the class `run`. In addition to its container function this class is used to normalize the signals with the emission current

and subtract the H₂ background (Sec. 5.3.1). The averaging for the calibration is also performed by the `signal` class.

The BRP and ABS model is implemented in a set of classes to model the signal based on the mode in which it was acquired. The `transition` class implements the HFTs transitions as matrices and defines the ABS and BRP mode names as enumerations. The `abs` and `brp` classes are inherited from `transition`. The `brp` class provides the functions $g_i(x; \beta_1, \beta_2, \dots, \beta_n)$ and $f_i(\mathbf{x}, \boldsymbol{\eta})$ discussed in Sec. 5.4 which are fed to the algorithms. The class also stores the calibration efficiencies and the hyperfine state population intensities. The `abs` class is mainly used to simulate or generate injection intensities either for a simulation or for a first approximation for the algorithms.

The algorithms and the linear algebra operators are implemented in the `vector` and `matrix` classes. All necessary linear algebra operators (e.g., addition, multiplication, vector product) and also the algorithms are implemented in a generic way. For example, the matrix equation

$$\mathbf{W} = (\mathbf{B} \mathbf{C} \mathbf{B}^T)^{-1}$$

is translated into¹: `la::matrix W = la::matrix::inverse(B*C*B.transpose());`

G.2. Usage of the Analysis Program

The program `brprun` is started from the command line and requires a command and a file name as arguments. The three main commands used for the polarization and calibration are: “process”, “cal” and “pol”. In all cases the raw data is always processed first with the “process” command. The processed signals are saved into two files:

$$\text{file.dat} \xrightarrow{\text{process}} \begin{cases} \text{file.dat.processed} \\ \text{file.dat.parameters} \end{cases}$$

one file contains the signals with errors and the respective acquisition mode and represents the minimal information for the polarization or calibration routines (extension “.processed”). The second file (with extension “.parameters”) contains the other parameters which were saved during the acquisition but which are not mandatory for the polarization or calibration. Per convention the raw data files have the extension “.dat”.

The calibration data is analyzed with the “cal” command and takes a processed file as input. The results are saved in a file with the same name as the input and the added extension “.results”:

$$\text{calibration.dat.processed} \xrightarrow{\text{cal}} \text{calibration.dat.processed.results.}$$

The results include the efficiencies, the intensities for all ABS modes and the covariance matrix C_e (see Eq. (5.10)).

The analysis of a polarization file is performed with the “pol” command. Each polarization run includes a reference to the calibration ID used during the measurement. This reference is crucial to be able to select the right calibration values. The calibration ID is the date of the calibration in the format YYYYMMDD. The program expects to find the calibration file named `calibration_results_YYYYMMDD.dat`. The results of the polarization measurements are written in the file “.results” and includes one run per line:

$$\text{polarization.dat.processed} \xrightarrow{\text{pol}} \text{polarization.dat.processed.results.}$$

¹the `vector` and `matrix` classes are declared in the namespace `la`.

The order and meaning of each data column is defined in the header. The raw data files which contain one day of acquisition can be concatenated and processed as a single file. The resulting file includes the polarization values for the whole period. All measurements lasting more than a day have been processed in this way (see Fig. 6.6). The “pol” and “cal” commands also accept a raw data file (with extension “.dat”), in this case the file will be automatically processed first.

The following commands show a step by step example of a calibration and polarization analysis.

```
./brprun cal ../data/cal_20100115.dat
cp ../data/cal_20100115.dat.processed.results calibration_results_20100115.dat
./brprun process ../data/polarization_20100130.dat
./brprun pol ../data/polarization_20100130.dat.processed
```

The last command produces the file `polarization_20100130.dat.processed.results` which contains all analyzed polarization runs.

A set of ROOT² macros is provided to visualize the polarization results. A single polarization measurement can be displayed with the macro `plot_hf_states.cpp`. It takes the polarization file and the run ID as arguments. The run ID is the time of the acquisition in the format `hhmmss`. If the run ID is not found, the next ID will be used. The Figs. 6.2 are created with this macro:

```
.x plot_hf_states.cpp("../data/pol_20100115.dat.processed.results",202818)
```

The polarization measurements of a full day or multiple days concatenated into one file are displayed with the `plot_polarization.cpp` macro. The “results” file is given as argument. This macro is used, for example, for Fig. 6.6:

```
.x plot_polarization.cpp("../data/pol_20100130.dat.processed.results")
```

²<http://root.cern.ch>.

H. PHYSICAL CONSTANTS AND NUMERICAL VALUES

Table H.1.: Physical Constants used in this diploma thesis [7, 140].

Quantity	Symbol, equation	Value
speed of light in vacuum	c	$299\,792\,458\,\text{m s}^{-1}$
Planck constant	h	$6.62606876(52) \times 10^{-34}\,\text{J s}$
Planck constant, reduced	$\hbar \equiv h/2\pi$	$1.054\,571\,596(82) \times 10^{-34}\,\text{J s}$ $= 6.582\,118\,89(26) \times 10^{-22}\,\text{MeV s}$
permittivity of free space	$\epsilon_0 = 1/\mu_0 c^2$	$8.854\,187\,817 \times 10^{-12}\,\text{F m}^{-1}$
permeability of free space	μ_0	$4\pi \times 10^{-7} = 12.566\,370\,614 \times 10^{-7}\,\text{N A}^{-2}$
fine-structure constant	$\alpha = e^2/4\pi\epsilon_0\hbar c$	$7.297\,352\,533(27) \times 10^{-3}$ $= 1/137.035\,999\,76(50)$
Avogadro constant	N_A	$6.022\,141\,99(47) \times 10^{23}\,\text{mol}^{-1}$
Boltzmann constant	k	$1.380\,650\,3(24) \times 10^{-23}\,\text{J K}^{-1}$ $= 8.617\,342(15) \times 10^{-5}\,\text{eV K}^{-1}$
electron charge magnitude	e	$1.602\,176\,462(63) \times 10^{-19}\,\text{C}$
electron mass	m_e	$0.510\,998\,902(21)\,\text{MeV}/c^2$ $= 9.109\,381\,88(72) \times 10^{-31}\,\text{kg}$
proton mass	m_p	$938.271\,998(38)\,\text{MeV}/c^2$ $= 1.672\,621\,58(13) \times 10^{-27}\,\text{kg}$ $= 1836.152\,6675(39)\,m_e$
deuteron mass	m_d	$1875.612\,762(75)\,\text{MeV}/c^2$
electron g-factor	g_e or g_s	$2.002\,319\,304\,362\,2(15)[140]$
proton g-factor	g_p	$5.585\,694\,713(46)$
deuteron g-factor	g_d	$0.857\,438\,2308(72)$
Bohr magneton	$\mu_B = e\hbar/2m_e$	$5.788\,381\,749(43) \times 10^{-11}\,\text{MeV T}^{-1}$
nuclear magneton	$\mu_N = e\hbar/2m_p$	$3.152451238(24) \times 10^{-14}\,\text{MeV T}^{-1}$
electron magnetic moment	$\frac{1}{2}g_s\,\mu_B$	$1.001\,159\,652\,193(10)\mu_B$
proton magnetic moment	$\frac{1}{2}g_p\,\mu_N$	$2.792\,847\,39(6)\mu_N$
deuteron magnetic moment	μ_d	$0.857\,438\,230(24)\mu_N$

Value	Hydrogen	Deuterium
ν_{HFS}/MHz	1420,405 751 768	327.384 352 51
E_{HFS}/eV	$5.874\,328\,324 \times 10^{-6}$	$1.353\,953\,384 \times 10^{-6}$
B_C/mT	50.683 622 91	11.681 890 93
$\epsilon_{H,D}$	$1.519\,270\,379 \times 10^{-3}$	$2.332\,033\,388 \times 10^{-4}$

Table H.2.: Hyperfine numerical values, the frequencies are measured with a high precision using masers [141, 85].

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Hiermit erkläre ich, dass ich die vorliegende Diplomarbeit selbständig erarbeitet und ausschließlich die aufgeführten Referenzen verwendet habe. Alle Quellen und Zitate sind als solche kenntlich gemacht, und die Literaturangaben sind nach meinem besten Wissen und Gewissen korrekt und vollständig wiedergegeben.