

# X-ray spectroscopy at PSI

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Crystal spectroscopy of the X-rays of exotic atoms started with a series of experiments using transmission spectrometers. Experiments at lower energies were made possible by the development of reflection spectroscopy. The progress made is illustrated with a measurement of the pion mass and the determination of strong interaction effects in pionic hydrogen isotopes. Modern developments aim at a determination of the strong interaction width on the level of %. The way to reach this goal is presented and the limits of the method and possible future experiments are discussed.

**Keywords:** exotic atom, X-rays, crystal spectroscopy

## 1. Introduction

This contribution tries to survey experiments at SIN/PSI where a high resolution crystal spectroscopy of X-rays emitted from excited levels of exotic atoms has been performed. Crystal spectroscopy makes use of the Bragg reflection of X-rays on crystals in order to compare the wavelength of radiation  $\lambda$  with the lattice spacing  $d$  of two crystal planes via the relation

$$n \lambda = 2d \sin \theta_B. \quad (1)$$

$n$  is the order of reflection.  $\theta_B$  is the angle of the incoming X-rays with respect to the crystal planes (Bragg angle) at which the reflections constructively interfere. As the lattice spacing is a well known quantity and angles can be measured with high precision, Bragg reflection offers a high potential to measure the energy of X-rays with high precision [1].

The basic features of exotic atoms are well described by the solution of the Dirac or the Klein–Gordon equation for a pointlike nucleus. A closer look, however, reveals deviations from this simple picture. The pure Coulomb interaction is disturbed by QED effects, the extended structure of the nucleus and the presence of the electron shell. Therefore particle physics as well as nuclear or atomic (molecular) physics aspects play a role in describing exotic atoms. The different fields of research can be attributed to different regions of principal quantum numbers. For low quantum numbers the overlap of the atomic wave function with the nucleus leads to the change of the energies which can be used to deter-

mine nuclear parameters in the case of muonic atoms and in special cases also for pionic atoms. The latter are mostly used to determine the strong interaction effect by measuring the induced shift and width of the atomic levels. Experiments at higher quantum numbers aim at the determination of the pion mass, the test of the validity of the Klein-Gordon equation or the search for anomalous interaction deviating from QED. They have to be carefully investigated whether electron screening shifts contribute. A part of the electron wave function shields the nuclear charge and hence leads to a smaller binding energy. This shift can not be calculated reliably as the status of the electron shell is not well enough known. For gaseous targets of low  $Z$  (below  $Z=10$ ) and a pressure of smaller than 100 hPa, however, complete ionisation has been proven [3]. The energies of the X-rays between principal quantum numbers higher than  $n=3$  are below 10 keV for these atoms and therefore only accessible to reflection spectrometers. The strongest motivation to use reflection spectrometers, however, came from a measurement of Lyman X-rays of pionic hydrogen atoms in the energy range between 2 and 3 keV.

The use of crystal spectrometers for the determination of the energies of the X-rays emitted during the cascade of the exotic atom increases the energy resolution compared to solid state detectors by orders of magnitude. As this increase implies a corresponding decrease of efficiency, the routine use of crystal spectrometers had to await the building of the high intensity meson factories. Even then special arrangements had been necessary to stop enough pions or muons. For muon spectroscopy a crystal spectrometer had been set up with an internal target in the cryogenic muon channel at SIN [4]. For the study of pionic atoms a novel method (Gatchina target) has been developed with the target in the vicinity of the pion production target [5,6]. Because of the bulky structure of the targets the energy of escaping X-rays was restricted in both cases to values higher than about 20 keV thus excluding the use of reflection spectrometers.

## 2. Experiments with transmission spectrometers

The two transmission spectrometers at SIN/PSI were used to study muonic atoms and interaction effects in pionic atoms. Both used the DuMond geometry with the need to scan the reflected X-rays.

### 2.1. Muonic atoms

The experiments at the muon channel at SIN concentrated on tests of the validity of quantum electrodynamics and on possible deviations from it as a search for so-called anomalous interactions [7,8]. In a measurement of the 2p-1s transitions in muonic carbon this also implied the determination of the root mean square radius of the carbon nucleus. The result represents the most precise value of this quantity and impressively demonstrates the possibilities of the exotic

atoms experiments. The transition energy of about 75 keV has been measured with a precision of 5.3 ppm. The achieved resolution was 4.9 eV. The root mean square radius of the  $^{12}\text{C}$  nucleus was determined to be  $2.4829 \pm 0.0019$  fm. This is a factor of about 2.5 more accurate than a suitable combination of 5 different results from electron scattering experiments. The measuring time of the experiment was 65 h at a proton current of  $70 \mu\text{A}$ . It should be mentioned that the corresponding total proton charge of 4.55 Cb is presently delivered in a time of less than one hour. The accuracy of the measurement, however, is limited by the nuclear polarization correction of 4 ppm.

In a similar experiment the 3d-2p transitions in muonic Mg and Si have been investigated. The transition energies had been determined with an accuracy of 2.9 ppm each. The vacuum polarization shift amounts to about 3000–4000 ppm of the transition energies. The result of the measurement represents the best determination of the vacuum polarization correction in bound states. The experiment was conducted at a mean proton current of  $70 \mu\text{A}$  with a total proton charge of 18.4 Cb for Si and 9.56 Cb in the case of Mg. The uncertainty from the electron screening correction is 2.1 ppm representing the limiting systematic error of the experiment.

## 2.2. Pionic atoms

The measurement of the mass of the negatively charged pion performed at the Gatchina target at SIN also met the difficulty represented by electron screening effects [9]. The position of the 4-3 transition in pionic magnesium was determined with an instrumental resolution of 0.93 eV. The observed line width was, however, about 20 % larger than the resolution and this was attributed to the occurrence of more than one configuration of the electron shell. Since each electron population causes a specific shielding of the nuclear charge, different electron screening shifts of the pionic transition energy occur which make the extraction of a value for the pion mass dependent on the different assumptions of the state of the electron shell.

In a different class of experiments the strong interaction shift and width of the 2p level in low Z pionic atoms were determined. The results corrected previous work with solid state detectors in an impressive way and served as a basis for further understanding of the p-wave pion nucleus interaction [10].

## 3. Experiments with reflection spectrometers

A new generation of experiments with reflection crystal spectrometers was based on several technical developments. These imply

- The intensity increase of pion beams. This is a result of both the intensity increase of the primary proton current in recent years and the setting up of the dedicated  $\pi\text{E5}$  beam at PSI.

- The cyclotron trap increased the stop densities by orders of magnitude and allowed to work with external targets avoiding the restrictions imposed by internal targets [2]. The decay of pions inside the cyclotron trap also produced a sufficient amount of muons stopping in the target.
- The development of cylindrically and spherically bent crystals with a size of the order  $100 \text{ cm}^2$ .
- The use of CCD detectors for the detection of low energy X-rays with excellent spatial and energy resolution. The spatial resolution was necessary to measure the reflex without time consuming scanning. It was moreover decisive to reduce the background caused by charged particles and X-rays of higher energies.

All these achievements made the use of external gas targets and the measurement of low energy X-rays feasible. The main application was the spectroscopy of the Lyman X-rays in pionic hydrogen isotopes to be discussed below. Moreover the spectroscopy of transitions between higher n-levels of low Z exotic atoms became accessible. In these atoms a high degree of ionisation had been demonstrated [3]. Interesting experiments could be conducted at pressures where the interaction of the exotic atom with the surrounding atoms was suppressed. This fact reduced or eliminated the electron screening problem as no electrons could be refilled from other atoms. Based on these achievements a new effort was started for a new determination of the pion mass.

### *3.1. Determination of the pion mass*

Because of the recent efforts in determining the mass of the muon neutrino a precision for the pion mass of the order of 1 ppm is required as the final accuracy of the result strongly depends on the knowledge of the mass of the charged pion [11]. A further motivation for a smaller error in the pion mass is the determination of the strong interaction effects in pionic hydrogen. The error in the calculation of the QED binding energies is mainly given by the error in the mass of the pion. It is also worth to mention that the accuracy in the calculation of the energy of undisturbed levels in exotic atoms is determined by the error in the pion mass. Nuclear masses have much smaller errors. Therefore a determination of the pion mass on the ppm level makes a new X-ray energy standard available. This is the more important as the transitions have a line width of less than 0.1 eV.

A new approach to determine the pion mass consisted in the direct comparison of the energies of muonic and pionic X-rays. It directly compares the mass of the pion with the muon mass which in turn had been determined for positive muons with a relative accuracy of 0.3 ppm. The simultaneous measurement of almost coinciding transitions in muonic oxygen and pionic nitrogen is free of most of the systematic errors. In a first round of the experiment the ability to stop enough pions in a gas target was demonstrated and a value for the pion mass could be extracted from a comparison with a Cu fluorescence line [12]. The ex-

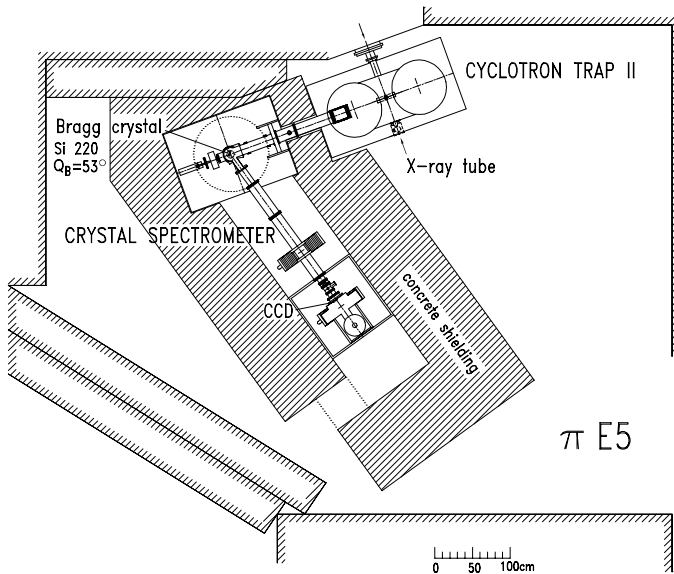


Figure 1. The Jülich reflection spectrometer at the  $\pi E5$  channel at PSI

perimental set-up typical for a reflection spectrometer is shown in Fig. 1. About  $4 \times 10^8$  negative pions were injected into the cyclotron trap per second at a proton current of 1 mA. Inside the target chamber of the cyclotron trap, a cylindrical target container with a diameter of 60 mm and thin walls ( $50 \mu\text{m}$  Kapton) was mounted. When this container was filled with nitrogen gas at one bar pressure, about  $10^6 \pi^-/\text{s}$  were stopped. The CCD detectors registered of about 120 pionic nitrogen X-rays/h with a peak/background ratio of 200:1. With a new cyclotron trap substantial improvements both in the number of stopped particles and in the reduction of background could be achieved. This led to the submission of a new proposal at PSI, which aims at a determination of the pion mass on the level of 1 ppm or better.

The experiment implies the simultaneous measurement of the pionic nitrogen and the muonic oxygen 4–3 transition at about 4 keV. A new CCD detector is being set up presently which is capable of having both the pionic and muonic transitions detected [13].

### 3.2. Strong interaction effects in pionic hydrogen

The pion–nucleon interaction is subject to experimental and theoretical studies since the very beginning of the development of particle physics. It is considered to be a fundamental problem of QCD. The understanding of strong interaction in the confinement regime has advanced recently, as chiral perturbation theory was developed to perform calculations at low energies [14–16]. In the framework of this theory the scattering lengths for pion nucleon scattering can

be calculated on the level of  $10^{-2}$ . The strong interaction shift and width of the ground state of pionic hydrogen are directly dependent on linear combinations of the two isospin separated scattering lengths. Therefore a precision measurement of both quantities should be performed. The measurement would in addition give a constraint to the phase shift analysis of the pion nucleon scattering experiments. As a third point the pion nucleon coupling constant could be directly extracted from the width measurement.

The shift and the width of the ground state in pionic hydrogen and deuterium have been determined in a series of experiments by the ETHZ-Neuchâtel-PSI collaboration by measuring the 3–1 transition at 2886 eV. The experimental set-up was very similar to the one shown in Fig. 1. An array of 6 cylindrically bent quartz crystals had been used in order to increase the statistics of the experiment. The pions were stopped with the help of the cyclotron trap I and the X-rays were detected with the Neuchâtel CCD detectors [17].

The results obtained represent an improvement by more than an order of magnitude compared to earlier work for the strong interaction shift. The experiment gave the first result for the width of the ground state [18]. At present the error in the width caused by Doppler broadening is almost an order of magnitude bigger than the one in the shift. This excludes the extraction of the isospin separated scattering lengths with errors on the %–level. The measurement is very useful, however, to put constraints on the different work in phase shift analysis of the scattering experiments in the pion nucleon system.

### *3.3. Proposed measurements of the strong interaction width in pionic hydrogen*

First tests with the newly designed cyclotron trap (cyclotron trap II) showed an enhancement in intensity by more than an order of magnitude and a further reduction of background (see Fig. 2) compared to earlier experiments.

As the intensity problem can be considered to be solved, the limitation in the determination of the strong interaction width is given by the Doppler effect caused by the so-called Coulomb deexcitation acceleration. In a recent proposal to PSI it is therefore planned to determine the ground state width (and shift) for the 2–1 (2433 eV) and the 3–1 (2886 eV) transitions at 3 different pressures between 3000 and 15000 hPa [19].

In a first step, however, it is planned to establish the independency of the ground state shift from pressure by measuring the energy of pionic 3–1 transition simultaneously to the pionic oxygen 6–5 transition at 2871 eV. The strong width is in a second step extracted from a simultaneous fit of the 6 transitions which keeps the different Doppler broadenings free but leaves the resolution for the different transitions fixed at its measured value. In addition the strong interaction width is assumed to be the same for all transitions. With this procedure a common value for the strong interaction width can be extracted with an accuracy of about 2.5%.

The still necessary increase in accuracy can be achieved by a simultaneous

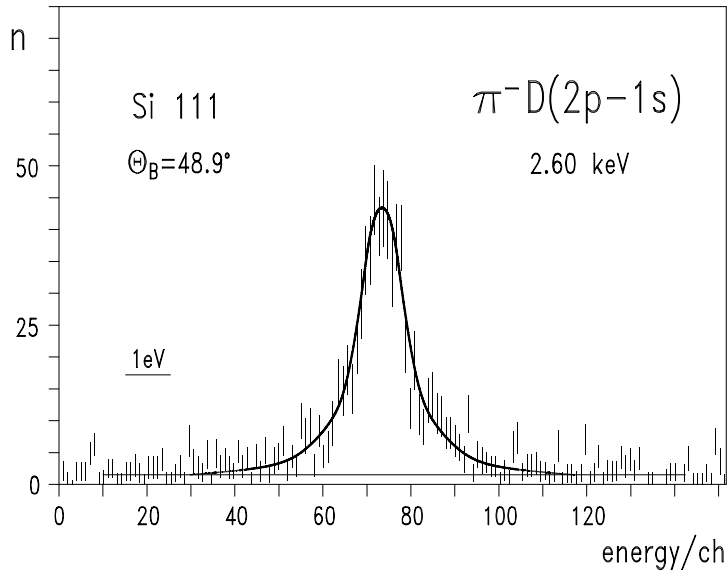


Figure 2. The 2-1 transition of pionic deuterium

spectroscopy of pionic and muonic hydrogen atoms in a third step of the experiment. The muonic X-rays do not show any strong broadening but exhibit a similar Doppler broadening as pionic atoms. In addition recent experiments determined the velocity state of the pionic hydrogen atom at the moment of the charge exchange reaction [20]. This together with the muon measurement constrains the input parameters for the calculation of the development of kinetic energies in the cascade of pionic hydrogen. The results of the cascade calculations can then be used to correct for the influence of the Doppler broadening.

#### 3.4. Combined measurement of muonic and pionic X-rays

For the newly proposed measurement a method was found to measure pionic and muonic X-rays simultaneously. This is made possible by the fact that the reduced masses of pionic and muonic hydrogen exhibit almost the same ratio as two lattice plane differences of quartz. With a two crystal set up one above the other the X-rays can be Bragg reflected to the same CCD detector. As an example a computer simulation of a hyperfine splitted muonic 2-1 transition is shown in Fig. 3. It comprises 20000 measured muonic X-rays which corresponds to a measuring time of 2 weeks at a pressure of 15 bar. The line is broadened by different contributions from Coulomb deexcitation process as calculated with a modern cascade program. A resolution of 220 meV is assumed for a quartz crystal. The peak to background ratio corresponds to recent experience.

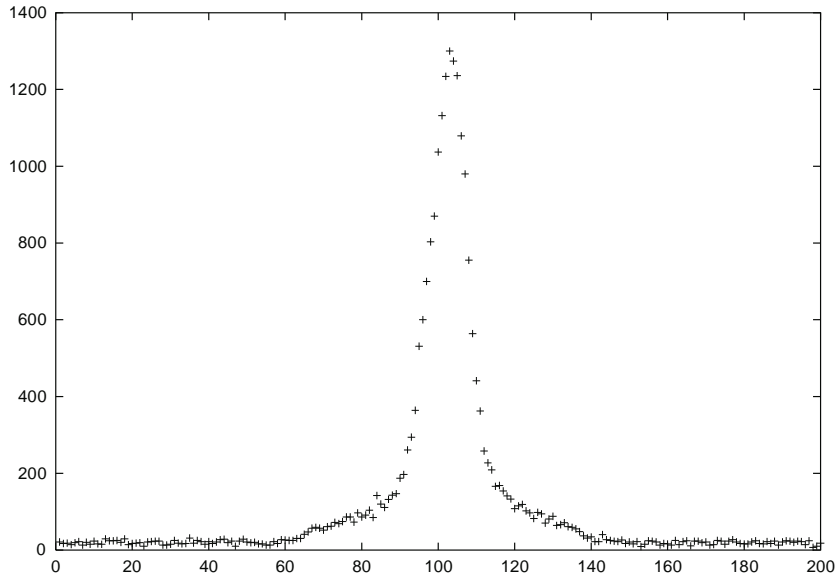


Figure 3. A simulation of the 2–1 transition in muonic hydrogen. The structure of the line reflects the different contributions from Coulomb deexcitation processes.

### 3.5. Calibration procedures

A successful X–ray spectroscopy of the quality required for the pionic hydrogen experiment bases on a narrow and well understood resolution function of the crystals. A calibration in energy or even an optimization can not be achieved with fluorescence X–rays as produced with X–ray tubes. Their width is an order of magnitude broader than the resolution of the crystals. The line shape is moreover influenced by not well determined satellite lines.

There are about 10 useful pionic transitions available in the region between 2000 and 3000 eV produced by the stopping of pions in low  $Z$  gases. Their rate, however, is not sufficient to do a time consuming optimization of the crystal resolution. A way out of this dilemma is granted by producing X–rays from one- or two–electron atoms. These can be produced copiously by electron cyclotron resonance (ECR) sources, which have been developed as ion sources for accelerators. The line width of the X–rays is determined almost exclusively by a very much reduced Doppler effect which leads to broadenings negligible compared to the intrinsic resolution of the crystals. Presently such a source is being set up at PSI. It is planned to test with it first with Si crystals of well understood response function. In a second step the response function of quartz crystals will be optimized and fluorescence sources will be calibrated. During the measurement with pions and muons the crystals can then be routinely surveyed with pionic X–rays which in turn can be used to energy calibrate the ECR measurement on the ppm level.



#### 4. Limitations of the method and possible new measurements

The Bragg reflection law itself directly hints at the limits of the crystal spectroscopy measurements. An error analysis gives

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \cot\theta_B \omega \quad (2)$$

$\omega = \Delta_B$  represents the intrinsic resolution of the crystal. The first term reflects the regularity of the crystal lattice over the extinction length. Optimal resolution requires to work at higher reflection orders where the extinction length is increased. For the (220) plane in Si the lattice plane difference has been determined with an error of  $3 \times 10^{-8}$  only [21], which means that special Si crystals show a macroscopic regularity of this degree. This fact could recently be exploited also for bent crystals using novel methods of crystal bending [22]. The second term contributes much more to the total error, as  $\omega$  is rarely below  $10^{-4}$ . It shows the necessity to work a high Bragg angles. Ideally the Bragg angle would be as near at 90 degrees as geometrically possible.

Moreover an analysis of the imaging errors for spherically bent crystals [23] shows a contribution from the extended size of the crystal to the accuracy in the wave length determination going with  $\cot^2\theta_B$ . The contribution from the height of the crystal is always negligible and the contribution from the height of the source can be corrected for. Two specific examples are selected to show the possibilities of new measurements at 90 degree Bragg angle.

##### 4.1. Determination of the vacuum polarisation in the 6-5 transition in muonic chlorine

The 6h-5g transition in muonic chlorine at about 9910 eV has a contribution from the vacuum polarization term of 4.5 eV compared to a fine structure splitting of 3 eV. The vacuum polarisation term in the satellite transition 6g-5f amounts to 8.1 eV with a fine structure splitting of about 6 eV. A measurement of 3.5 eV for the difference of the energies of the circular transitions compared to their satellite lines would be a direct measure of the vacuum polarisation term. The fine structure splittings then serves as a calibration. The energy complex is in reasonable neighbourhood to the 90 degree value for the reflection at the Si(555) plane which has an energy at 9885 eV. The Bragg angle for the muonic lines is at 85.9 degrees with  $\cot\theta_B = 0.0711$ . An energy resolution of 15 meV can be reached, which would result in a determination of the vacuum polarisation contribution on the level of 100 ppm provided 1000 entries can be registered in the satellite transition.

#### 4.2. Determination of the Lamb shift contribution in electronic chromium

The energy of the Lyman transitions at about 5932 eV corresponds almost exactly to the minimum energy which is Bragg reflected at the Si(333) plane. The Bragg angle is 89.04 degree which corresponds to  $\cot \theta_B = 0.0157$ . An energy resolution of 53 meV can be reached which allows to reach an accuracy of  $10^{-3}$  for the Lamb shift measurement. A suitable ECR source can provide enough intensity. The measurement would require an absolute measurement of the Bragg angle on the level of precision of  $10^{-7}$ .

### 5. Conclusions

Crystal spectroscopy of X-rays from exotic atoms has reached a resolution of about  $10^{-4}$  for reflection spectrometers. This allows to extend the measurements to exotic hydrogen isotopes in order to test the predictions of the chiral perturbation theory of strong interaction. Special arrangements with Bragg angles slightly lower than 90 degrees can suppress systematic errors and may open a new window for a sub ppm level of energy measurements. A determination of the pion mass with an accuracy of 1 ppm (or better) delivers a new energy standard.

### References

- [1] D. Gotta, contribution to this workshop.
- [2] L. M. Simons, *Phyjsica Scripta* T22 (1988) 90; *Hyperfine Interactions* 81 (1993) 253.
- [3] R. Bacher et al. *Phys. Rev. A*39(1989) 1610.
- [4] W. Beer, P.F.A. Goudsmit and L. Knecht, *N.I.M.* 219 (1984) 322.
- [5] V. I. Marushenko et al., *JETP Lett.* 23 (1976) 72.
- [6] W. Beer et al., *N.I.M.* A238 (1985)365.
- [7] W. Ruckstuhl et al. *Nucl. Phys.* A430(1984)685.
- [8] W. Ruckstuhl et al. *Nucl. Phys.* A433(1985)634.
- [9] B. Jeckelmann, P.F.A. Goudsmit, H. J. Leisi, *Phys. Lett.* B335(1994)326.
- [10] G. de Chambrier et al. *Nucl. Phys.* A442 (1985) 637.
- [11] K. Assamagan et al., *Phys. Rev. C*53(1996) 6065.
- [12] S. Lenz et al. *Phys. Lett.* B416 (1998)50.
- [13] PSI proposal R-97-02.1
- [14] J. Gasser and H. Leutwyler, *Phys. Rep.* 87C (1982) 77.
- [15] E. Jenkins and A.V. Manohar, *Phys. Lett.* B255 (1991) 558.
- [16] J. Gasser and H. Leutwyler, *Ann. Phys. (N.Y.)*158 (1984) 124.
- [17] J.P. Egger, contribution to this workhop.
- [18] D. Sigg et al., *Nucl. Phys.* A609 (1996) 269.
- [19] PSI proposal R-98-01.1
- [20] Publikation Daum and contribution to this workshop.
- [21] G. Basile et al., *Phys. Rev. Lett.* 72 (1994) 3133.
- [22] G. Masciovecchio et al. *N.I.M.* B111 (1996)181.
- [23] J. Eggs and K. Ulmer, *Zeitschrift für angewandte Physik* 20 (1965) 118.