Crystal Spectroscopy and Exotic Atoms

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Abstract. Recent developments in crystal spectroscopy of X-rays emitted from exotic atoms concentrated on the measurement of the ground state level shift and width in pionic hydrogen. An increase of the pion beam intensity together with a sophisticated stopping technique combined with newly developed reflection spectrometers as well as with large area focal CCD detectors resulted in a gain of luminosity of three orders of magnitude. The potential of these achievements for an improved measurement of the vacuum polarization contribution in exotic atoms is discussed.

INTRODUCTION

High resolution crystal spectroscopy of X-rays emitted from muonic or pionic atoms has been a substantial part of the experimental program at SIN/PSI for the last two decades. The experimental method makes use of the Bragg reflection of X-rays on crystals in order to compare the wavelength of radiation λ with the lattice spacing d of two crystal planes via the relation

$$n\ \lambda = 2d \sin\theta_B, \tag{1}$$

where n is the order of reflection and θ_B is the angle of the incoming X-rays with respect to the crystal planes (Bragg angle) at which the reflections constructively interfere. As angle differences can be measured very precisely, Bragg reflection offers a high potential for the determination of differences of X-ray energies.

Exotic atoms offer many possibilities for a high precision spectroscopy, which 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 changes in binding energies energies, which can then be used to determine nuclear parameters as it was done extensively in the case of muonic atoms. Pionic atoms are mostly used to determine strong interaction effects by measuring the induced shift and width of the atomic levels. Experiments on levels with higher quantum numbers aim at the determination of, e.g., the pion mass, at testing higher order QED

calculations or at the search for anomalous interactions leading to deviations from QED. Such experiments have to be carefully investigated to check whether electron screening shifts may lead to smaller binding energy, which are uncontrollable as the status of the electron shell is not exactly known. In fact the electron screening contribution limited the accuracy of most of the crystal spectrometer experiments done in past with transmission spectrometers. For gaseous targets below $Z = 18$ and a pressure of lower than 0.1 bar, however, complete ionization has been established for muonic (pionic) atoms [1]. 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.

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

- The intensity increase of pion beams. This is a result of both the intensity increase of the primary proton current by a factor of more than ten in recent years and the setting up of the dedicated πE5 pion channel at PSI.
- A superconducting split coil magnet (cyclotron trap) increased the stop densities by two orders of magnitude for pions and allowed to work with external targets [2]. The decay of pions inside the cyclotron trap also produced a sufficient amount of stopped muons.
- The development of cylindrically and spherically bent crystals with a size of the order of 100 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 decisive also to reduce the background caused by charged particles and X-rays of higher energies [3].

PIONIC HYDROGEN

The understanding of strong interaction in the confinement regime has advanced recently, as chiral perturbation theory was developed to perform calculations at low energies [4].

Its extension to heavy baryon chiral perturbation theory [5] allows to calculate many of the experimentally accessible processes in the meson nucleon sector. The check of the soundness of this approach requires high precision experiments. This resembles the situation in the development of QED during the last 50 years, where the measurement of the Lamb shift contributed much to the development of QED. In a comparable way the measurement of strong interaction shift and width in pionic hydrogen can be considered to be a key experiment in strong interaction physics at low energies.

This atom is dominated by the electromagnetic interaction of its constituents. Their strong interaction is only effective if the wave functions of pions and the

proton significantly overlap. In the ground state it results in a broadening of $\approx 1\ eV$ and a shift of $\approx 7\ eV$, which has to be compared to an electromagnetic binding energy of $E_{1s} = 3238\ eV$. The relations of the measured quantities to the hadronic scattering lengths a^h describing the $\pi^- p \to \pi^- p$ and the $\pi^- p \to \pi^0 n$ process, respectively, are given by the Deser-type formulae [6,7]:

$$\frac{\epsilon_{1s}}{E_{1s}} = -4\frac{1}{r_B} a^h_{\pi^- p \to \pi^- p}(1 + \delta_\epsilon) \tag{2}$$

$$\frac{\Gamma_{1s}}{E_{1s}} = 8\frac{Q_0}{r_B}(1 + \frac{1}{P})(a^h_{\pi^- p \to \pi^0 p}(1 + \delta_\Gamma))^2 \tag{3}$$

Here r_B is the Bohr radius of the pionic hydrogen atom with $r_B = 222.56$ fm, $Q_0 = 0.142\ fm^{-1}$ is a kinematical factor and P=1.546±0.009 is the Panofsky ratio [8]. δ_ϵ and δ_Γ are electromagnetic corrections, which have recently been calculated with a potential model with an accuracy of about 0.5% [9]. In a recent study the problem of the electromagnetic corrections is discussed and the potential model ansatz is critisized [10].

The relations of the measured quantities with the isospin separated scattering lengths b_0 (isoscalar) and b_1 (isovector) are given by:

$$a^h_{\pi^- p \to \pi^- p} = b_0 - b_1 \tag{4}$$

and

$$a^h_{\pi^- p \to \pi^0 p} = \sqrt{2} b_1 \tag{5}$$

The shift and the width of the ground state in pionic hydrogen and deuterium have been determined in a series of experiments of the ETHZ-Neuchâtel-PSI collaboration by measuring the 3–1 transition at 2886 eV with a reflection type crystal spectrometer [11].

The results improved the value for the strong interaction shift by almost two orders of magnitude compared to earlier work. In addition first results for the width of the ground state were obtained. The error in the width, however, is still almost an order of magnitude bigger than the one in the shift and is strongly influenced by the poor knowledge of accelerating mechanisms during the de-excitation of the atom. The acceleration results in different contributions of Doppler broadening of the X-ray energy. This excludes the extraction of the isospin separated scattering lengths with errors on the %–level from the hydrogen experiment alone.

An illustration of the most recent evaluations for b_0 and b_1 from atomic data as well as from scattering data is shown in Figure 1. The data from scattering experiments lead to the bands limited by full lines. They have been obtained by critically investigating the different cross sections for the $\pi^+ p$ (proportional to $b_0 + b_1$), and $\pi^- p$ (proportional to $b_0 - b_1$) and charge exchange processes (proportional

to b_1) and extrapolating them to zero energy [12]. All three bands from the different linear combinations of b_0 and b_1 coincide in a narrow region in the (b_0, b_1) plane with corresponding values of about $b_1 = -0.082 m_\pi^{-1}$ and $b_0 = 0.003 m_\pi^{-1}$ each with errors of about $\pm 0.001 m_\pi^{-1}$. As the three different constraints originate from many different sets of experiments, the common intersection can be considered as a quite impressive result. Some criticism was expressed, however, concerning the validity of the model used [13]. It should be mentioned that earlier evaluations of scattering data lead to quite different results [14,15]. Especially the value of $b_0 + b_1$ extracted from the Karlsruhe-Helsinki evaluation with a value of $-0.101 m_\pi^{-1}$ contradicts the evaluation mentioned above which assumes $b_0 + b_1 = -0.077 \pm 0.002 m_\pi^{-1}$

The data from pionic atoms lead to the regions limited by the dashed lines. As stated before the large error in the width measurement precludes an extraction of b_0 and b_1 with sufficient precision. Moreover the band resulting from the shift measurement alone is at variance with the corresponding $\pi^- p$ scattering data. A recent evaluation of pionic deuterium shift data results in a a small overlapping area if combined with the pionic hydrogen shift data [16]. The results in terms of scattering lengths are $b_0 = -0.0017 \pm 0.001 m_\pi^{-1}$ and $b_1 = -0.09 \pm 0.0012 m_\pi^{-1}$. An evaluation of the ETHZ-PSI-Neuchatel group using earlier theoretical input for the evaluation of the deuterium data resulted in almost the same value for b_0 but gave

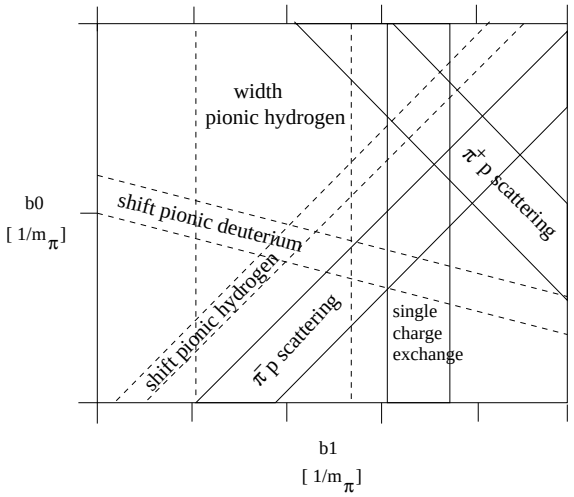

FIGURE 1. Information on b_0 and b_1 from scattering experiments and exotic atom data.

a somewhat different value of $b_1 = -0.0868 \pm 0.0014 m_\pi^{-1}$ [17].

In conclusion it can be stated that the results from scattering data and atom experiments are still contradictory and therefore need further investigation. From the side of the atom experiments it should be clarified whether the shift and the width values of pionic hydrogen and deuterium are true strong interaction effects and are not spoiled by the interaction of the pionic atom with the surrounding molecules.

In a recent proposal to PSI it is planned to determine the ground state width (and shift) from the 2–1 (2433 eV) and the 3–1 (2886 eV) as well as the 4–1 (3042 eV) transitions at several pressures between 3 and 15 bar [18].

In a first step of the experiment, the width can be extracted from a simultaneous fit of all transitions, which lets the different Doppler broadenings free, but keeps the response function for the different transitions fixed at its independently determined value. Using the fact that the strong interaction width is the same for all transitions, a common value for the strong interaction width can be extracted with an accuracy of about 2.5%.

The still necessary increase in accuracy requires an additional effort. A simultaneous spectroscopy of pionic and muonic hydrogen atoms is planned as the muonic X-rays do not show any strong interaction broadening, but exhibit Doppler broadening similar to pionic atoms.

VACUUM POLARIZATION IN EXOTIC ATOMS

Now the question will be considered whether an improvement of the present accuracy of 900 ppm in the vacuum polarization (VP) contribution to the binding energy in exotic atoms can be achieved. Tests of QED in electronic hydrogenlike ions have provided values for the Lamb shift of at best a few %. As vacuum polarization is only a small contribution of the total Lamb shift (from 0.2% in hydrogen to 20% in hydrogenlike uranium), exotic atoms offer a unique possibility of studying objects in which vacuum polarization heavily dominates. It means that higher-order corrections like three-loop vacuum polarization, which are completely negligible in electronic atoms, are relevant. The size of the contributions to the transition energy for two examples are shown in Table 1. Because the Bohr radius in pionic or muonic atoms is more than 200 times smaller than in normal atoms, one is then more sensitive to short distance interactions. Finally, pions being spin 0 bosons, the fine structure of pionic atoms enables to test in details the Klein-Gordon equation. For an optimum experiment a proper choice of transition and target element is in order: The transition should not be influenced by nuclear effects (finite size, nuclear polarization) and on the other hand electron screening and line broadening effect (Coulomb explosion of molecules) should be avoided. The latter requirements restrict the choice to mono-atomic (or equivalent) gaseous targets with Z lower than 18. In order to have a sizeable contribution of the vacuum polarization term the choice should try to maximize Z and minimize the principal

TABLE 1. Contributions to the transition energy of $\pi\,^{14}\mathrm{N}^{7+}$ and $\pi\,^{40}\mathrm{Ar}^{18+}$, with energies around 8 keV (eV).

Element	^{14}N, $4f-3d$	^{40}Ar, $7i-6h$	Diff.
Klein-Gordon (fin. nucl.)	8759.815	8842.728	-82.913
Uehling ($\alpha Z\alpha$)	8.223	3.669	4.553
Wichman and Kroll ($\alpha(Z\alpha)^3$)	-0.003	-0.013	0.010
Källén and Sabry ($\alpha^2 Z\alpha$)	0.066	0.034	0.032
Loop after loop Uehling ($\alpha^2 Z\alpha$)	0.010	0.003	0.007
Relat. recoil	0.011	0.007	0.004
Total	8768.122	8846.429	-78.307

quantum number of the transition, i.e., the energy should be at a maximum. This meets the requirement from the side of the detection technique which gives best resolution for higher energies. A limit is given by the rapidly dropping efficiency of the CCD detectors above 10 keV. As an order of magnitude more pions than muons can be stopped in thin targets, pionic atoms are considered preferentially. In this case the influence of strong interaction shifts deserves special attention.

The VP shift for the cases to be studied is at the best on a level of 1000 ppm of the transition energy. Aiming at a relative accuracy of 100 ppm in the VP term requires an energy determination on the level of 0.1 ppm. This is far beyond the present possibilities of doing absolute energy measurements with bent crystal spectrometers and even an an order of magnitude less than the present knowledge of the pion mass. Relative energy measurements, however, are not excluded. They rely on a comparison of transitions with almost identical Bragg angles but with VP contributions as different as possible. These can be the comparison of circular and parallel transitions for the same element or a comparison of circular transitions of two different elements. Here it should be kept in mind that parallel transitions have an intensity of about 10% of the circular transition, but also that the number of muon stops presently achieved is an order of magnitude less compared to pions.

Circular and parallel transitions for one Z

The VP contribution of a parallel transition has almost the double value of the circular transition. An illustrative case is the 5–4 transitions in pionic ^{20}Ne. The circular transition $5g-4f$ has an energy of 8306.4485 eV with a 5.4483 eV contribution of higher order QED effects, mainly vacuum polarization. The parallel $(5f-4d)$ transition is higher in energy by 8.8731 eV with a VP contribution of 9.8096 eV. The QED difference of about 4.361 eV should be determined with 0.4 meV accuracy. The $4d$ state is affected by strong interaction shift on the level of less than 0.1 meV. The dispersion calibration as well as a control of systematic errors is provided by overlapping the same transitions from ^{22}Ne by working with an 50:50 mixture of the two isotopes. The circular transition of ^{22}Ne is shifted to higher energies by 5.6292 eV compared to ^{20}Ne (5.6354 eV for the parallel transition). As

a result the parallel transition of ^{20}Ne is only 1.2432 eV higher in energy as the circular transition of ^{22}Ne.

The experiment would be conducted at a target pressure of typically 10 bar, eventually in a mixture with hydrogen in order to maximize the yield of the parallel transition. The yield of the parallel transition can be expected to be at least 5% with a rate of about 40/h. A flat crystal rocking curve width of 40 meV for the Bragg reflection of Si (444) would result in a measuring time of 2 weeks in order to reach a 100 ppm accuracy in the VP contribution. Bending the crystals results in a considerably worse width from the geometry (Johann broadening) only [19] which together with effects from crystal distortion excludes the abovementioned measurement at present time.

Circular transitions of different elements

The $7i - 6h$ transition in pionic argon is 78.307 eV higher in energy than the $4f - 3d$ transition in pionic nitrogen at 8768.121 eV. The difference in the vacuum polarization of both transitions is 4.506 eV. Working with a mixture of 50% NH_3 to 50% Ar at a pressure of 2 bar an event rate of about 500/h can be expected for both transitions. With a theoretical line width of 40 meV for the Si (444) reflex (mean Bragg angle 63.9^o) a statistical accuracy of 100 ppm can be expected in 1 day of measurement. The distance of the two lines is about 54 mm which would require a target broader than used routinely as well as a broader CCD detector. Choosing the Si (440) reflection would result in an acceptable distance of 28 mm between the two lines with a still tolerable resolution of 80 meV. Then also the Si $6h - 5g$ transition (with SiH_4 as target gas) which is about 92 eV higher in energy than the nitrogen transition could be measured to provide an independent check. Geometrical broadening caused by bending the crystal results in a factor of four worse resolution if the same rate should be maintained. Even then the experiment would be feasible in a convenient time.

Bragg angles near 90^o

An analysis of the imaging errors for spherically bent crystals shows a contribution from the width of the crystal, which influences the accuracy in the wave length determination with a term proportional to $\cot^2\theta_B$. The contribution from the height of the crystal is always negligible and the contribution from the height of the source can be corrected for. Hence experiments should be considered, which allow an observation a large Bragg angles.

One example is the determination of the vacuum polarization in the 6–5 structure in muonic chlorine. The $6h - 5g$ transition in muonic chlorine at about 9912 eV has a vacuum polarization contribution of 4.4 eV compared to a fine structure splitting of 3 eV. The vacuum polarization term in the parallel transition $6g - 5f$ amounts to 8.05 eV with a fine structure splitting of about 5.5 eV. An accurate

determination of the 3.6 eV difference in energy of the two parallel transitions measures the vacuum polarization term directly. The fine structure splittings as well as isotope transitions serve as dispersion calibration. The energy complex is in reasonable neighborhood to the 90^o 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^o with cot $\theta_B = 0.0711$. An energy resolution of 15 meV can be reached, which would result in a determination of the VP contribution on the level of 100 ppm provided 1000 events can be registered in the satellite transition. In order to achieve this a set-up of the cyclotron trap at a dedicated muon beam should be chosen.

CONCLUSIONS

Crystal spectroscopy of X-rays from exotic atoms developed considerably during the last decade in order to test the predictions of the chiral perturbation theory of strong interaction in precision measurements of X-rays in hydrogen isotopes. The present state of technology can be used to determine the VP contribution in special exotic atoms with an order of magnitude increased precision.

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