

Kinetics of atomic cascade in pionic hydrogen

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The new pionic hydrogen shift/width experiment at PSI [1, 2] aims at obtaining the strong interaction width of the ground state of π^-p with a precision better than 2%. Reliable procedures for subtracting the Doppler broadening corrections from the measured $np \rightarrow 1s$ X-ray line profiles must be applied. We discuss the acceleration mechanisms responsible for the high energy (several tens of electron–Volts) π^-p atoms and which constraints may be imposed on the kinetic energy distributions.

1 Doppler broadening of the X-ray lines in pionic hydrogen

The Pionic Hydrogen Collaboration [1, 2] has measured the X-ray line profiles of the $2p \rightarrow 1s$, the $3p \rightarrow 1s$, and the $4p \rightarrow 1s$ transitions in π^-p at different densities. Each measured profile, P , is a convolution of three functions

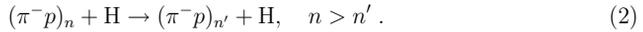
$$P = L \otimes D \otimes R \tag{1}$$

where L is a Lorentzian with width $\Gamma_{1s}^{\text{had}} \sim 800$ meV, D the Doppler broadening correction and R the resolution function. That the Doppler broadening of the X-ray lines is large was demonstrated by the different widths (after subtraction of the resolution function) that were measured for the transitions in 2002 at 10 bar [3]: the width of the $2p \rightarrow 1s$ transition was found to be more than 200 meV larger than that of the $4p \rightarrow 1s$ transition indicating more energetic π^-p atoms at the $n = 2$ level.

The analysis of the experiment is based on a fitting procedure aimed at determining the unknown strong interaction width, Γ_{1s}^{had} , and 2–4 parameters for each transition describing the kinetic energy distribution [1]. The more constraints one can impose on the kinetic energy distributions, the more accurate the final value for Γ_{1s}^{had} will be. A good understanding of the kinetics of atomic cascade in pionic hydrogen is, therefore, required.

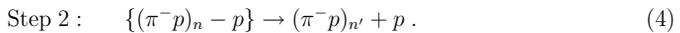
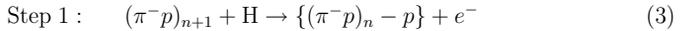
2 Acceleration mechanisms

It has been known for some time that exotic hydrogen atoms (μp , $\pi^- p$, $K^- p$, etc.) can reach kinetic energies of several tens of electron–Volts during the atomic cascade [4]. The most straight–forward way of gaining substantial kinetic energy is through direct Coulomb deexcitation [5]:



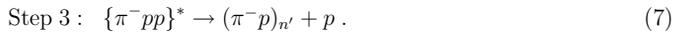
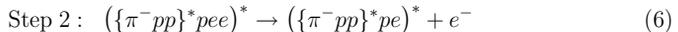
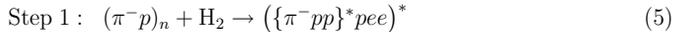
In this process, the released energy from the transition $n \rightarrow n'$ is shared between between the $\pi^- p$ and the H atom. This results in $\pi^- p$ high energy components with characteristic kinetic energies: 34 eV for the $5 \rightarrow 4$ transition, 73 eV for $4 \rightarrow 3$, and 209 eV for $3 \rightarrow 2$.

A slightly more involved process is Coulomb deexcitation via Auger capture [6]:



Here the $\pi^- p$ atom ends up in a weakly bound state with the target proton after ionization. Step 2 will result in lower kinetic energies than the direct Coulomb deexcitation. Of course, nuclear absorption instead of Coulomb deexcitation is also possible.

A third process requires a H_2 target in order to absorb excess kinetic energy [7]:



Contrary to the direct Coulomb deexcitation, several different kinetic energies are possible in the final state. The $\{(\pi^- pp)^+\}$ molecular ion has a number of resonances below the $n = 2, 3, 4$ thresholds [7, 8]. For example, the lowest–lying resonance below the $n = 4$ threshold is a 1S state with the energy -68.1 eV relative to the free $(\pi^- p)_{n=4} - p$ system. After break–up, the $(\pi^- p)_{n=3}$ atom will have the kinetic energy ~ 41.5 eV which is substantially less than the 73 eV in case of direct Coulomb deexcitation.

3 Constraints on the kinetic energy distributions

It is crucial for the extraction of the $1s$ width that some constraints are imposed. If not, only an upper limit for Γ_{1s}^{had} can be obtained because the whole broadening could in principle be due to a particular kinetic energy distribution (so that $\Gamma_{1s}^{\text{had}} = 0$). Based on our present knowledge one can try to

- Impose upper energy limits.
- Determine other kinetic energy ranges where no $\pi^- p$ atoms are expected.
- Use the fact that the kinetic energy distributions for the different $np \rightarrow 1s$ transitions are inter–dependent.

Imposing upper limits on the kinetic energy is probably the most important constraint. If $\Delta n > 1$ Coulomb transitions at low n are negligible compared to $\Delta n = 1$ transitions, the upper limits are ~ 209 eV, ~ 73 eV, and ~ 34 eV for $n = 2, 3, 4$, respectively. The ongoing analyses with only these constraints are very promising [1].

If molecular states play a negligible role for the acceleration of the π^-p atoms, the kinetic energy distribution at the instant of the $3p \rightarrow 1s$ transition could look like Fig. 1.

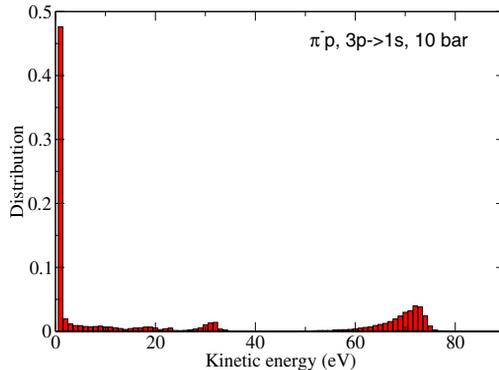


Figure 1: The kinetic energy distribution at the instant of the $3p \rightarrow 1s$ transition as predicted by the ESCM.

The figure shows the prediction of the extended standard cascade model (ESCM) [9, 10] which does not include the molecular process. One notices the $4 \rightarrow 3$ Coulomb component at ~ 73 eV and the $5 \rightarrow 4$ Coulomb component at ~ 34 eV. Though the prediction of the weights of the high energy components is uncertain (as compared to what is required by the experiment) some general features could be used in the fitting procedure – notably that the distribution is nearly zero in the range 35–55 eV.

The kinetic energy distributions in π^-p at the instant of the different $np \rightarrow 1s$ transitions are related to each other. For example, the 73 eV component appearing at $n = 3$ will contribute to the Doppler broadening of both the $3p \rightarrow 1s$ and $2p \rightarrow 1s$ line. Though the absolute weights of this high energy component in the two spectra are difficult to calculate, once it is determined by the fitting procedure in one spectrum the weight in the other spectrum can be predicted. The accuracy of the prediction depends on having reliable cross sections for the collisional processes at $n = 2, 3$ at high energies. It is independent of the cascade processes at low energies and $n > 3$ which are not well understood.

A cascade model dealing only with the high energy components in the final part of the π^-p cascade has been written, see Fig. 2. The Stark transitions [9, 10, 11]



are very important because they modify the population of the nl substates at a given level n which in turn determine the relative importance of nuclear absorption (from the ns states) and the X-ray transitions.

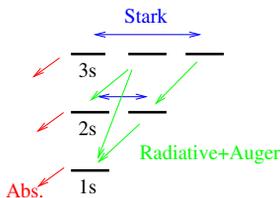


Figure 2: Cascade model for the high energy components in the final part of the cascade. The π^-p atoms deexcite via radiative transitions and the external Auger effect while Stark transitions change the population of the nl substates and lead to nuclear absorption.

The cross sections for the Stark transitions have been calculated for atomic target (fully quantum mechanical close coupling model (CC) and the semiclassical straight-line-trajectory approximation (SLTA)) and molecular target (SLTA). The SLTA is a good approximation at high energies: for $n = 3$ and $E_{\text{kin}} = 73$ eV the cross sections calculated for atomic target are given in Table 1.

Process	CC	SLTA
$3p \rightarrow 3s + \text{abs.}$	0.674	0.688
$3p \rightarrow 3d$	1.547	1.544
$3d \rightarrow 3s + \text{abs.}$	0.186	0.182
$3d \rightarrow 3p$	0.928	0.927

Table 1: The cross sections (in a_0^2) for π^-p with kinetic energy 73 eV scattering from hydrogen atoms [11].

In the case of molecular target the calculation of the Stark cross sections is done assuming the H_2 molecule (including electronic density) to remain fixed during collision and averaging over the spatial orientations [11]. In the cascade model one can calculate the fractions of a given high energy component which are absorbed at $n = 2, 3$ or go through the different X-ray transitions. The results for the 73 eV component at 10 bar for molecular and atomic target are given in Table 2. The results show that 73% of these high energy π^-p atoms experience nuclear absorption at $n = 2, 3$ (for molecular target) while 27% give rise to K X-rays. The predicted yield ratio, $Y(K_\alpha)/Y(K_\beta)$, puts constraints on the kinetic energy distributions at $n = 2$ and $n = 3$ and can be used by the fitting program [1] to reduce the number of free parameters.

Yield	Molecular	Atomic
$Y(K_\alpha)$	10.7%	8.7%
$Y(K_\beta)$	16.3%	13.8%
Absorption	73.0%	77.5%
$Y(K_\alpha)/Y(K_\beta)$	0.659	0.627

Table 2: The calculated X-ray yield and absorption fractions at 10 bar from the high energy component created at $n = 3$ with 73 eV.

4 Conclusion

- The extraction of the $1s$ strong interaction width in pionic hydrogen from measured X-ray profiles requires a good understanding of the kinetics of atomic cascade.

- Ab initio calculations of kinetic energy distributions do not reach the required accuracy for the pionic hydrogen shift/width experiment.
- However, there are constraints which can be imposed on the distributions and hence reduce the number of free parameters in the fitting procedure used for extracting the $1s$ width.
- The measured line profile in muonic hydrogen and future high statistics measurements in pionic hydrogen should lead to a clarification with respect to relative importance of the different acceleration processes during the atomic cascade.

Acknowledgment. This work was supported by the Swiss National Science Foundation.

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