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Testing the ECPSSR theory and its modifications with ratios of antiproton-to-proton ionization cross sections

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Abstract

While fits to 90% of all ever measured K-shell ionization cross sections by protons are on the average within 10% of the ECPSSR [W. Brandt, G. Lapicki, Phys. Rev. A 23 (1981) 1717], this theory systematically overestimates the remaining 10% of all data (comprised mainly of the measurements on heavy target elements) in the slow collision regime of proton velocities less than 0.1 of the orbital velocity of the K-shell electron. For ionization of H and He, experimental ratios of antiproton-to-proton cross sections and benchmark theories thereof exist in the range around where the projectile and target electron velocities match and the cross sections peak. They confirm the excellent accuracy with which the antibinding/binding and antipolarization/polarization effects are accounted for in the perturbed-stationary state (PSS) treatment of the ECPSSR theory. It is shown that the K-shell ionization of *heavy* elements by MeV antiprotons, which were routinely extracted from the LEAR – or alternatively in ionization of light elements below 0.3 MeV that will become available at the GSI's future Facility for Low-Energy Antiproton and Ion Research (FLAIR) – would provide for a decisive and critical test between various modifications of the ECPSSR theory and any other theory of inner-shell ionization by protons and antiprotons.

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Keywords: Ionization; Protons; Antiprotons; K-shell; ECPSSR theory

1. Introduction

Over two decades ago, to set up a benchmark for perturbative theories that go beyond the first-order Born approximation such as the ECPSSR theory [1], Reading and coworkers supplemented their earlier close-coupling calculations

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for ionization of atomic hydrogen by protons [2] with a similar calculation for antiprotons [3]. Spurred by the then emerging programs at the CERN's Low-Energy Antiproton Ring (LEAR), Brandt and Basbas [4] – based on antibinding versus binding and antipolarization versus polarization effects in the perturbed-stationary state (PSS) treatment of the ECPSSR theory – calculated the ratios of K-shell ionization cross sections in $_{13}$Al for 0.004–4 MeV antiprotons and protons to be above 0.4 MeV larger and smaller than 1, respectively, at lower and higher energies. As the energy decreased below 0.4 MeV, the PSS effects were overshadowed due to the divergent trajectories in which protons and antiprotons are repelled and attracted in the Coulomb field of the target nucleus. In accordance with the Coulomb deflection factor of the ECPSSR theory, cross sections for ejection of the K-shell electron into the continuum by protons and antiprotons, respectively, decline and grow exponentially; hence the antiproton-to-proton ratio for K-shell ionization in aluminum rose dramatically to a factor of 1000 at 0.04 MeV. Reading's 1984 quest for progress "in sorting out the inaccuracies" [5] in the ECPSSR theory would be fully (i.e. for a test of the Coulomb deflection factor and the binding effect function converging to the proper united atom value in the slow collision limit) possible if one could reliably calculate or measure ionization cross sections with keV-antiprotons for hydrogen and the lightest elements or with MeV-antiprotons for inner-shell ionization cross sections for heavy target atoms. Although, as of the 1992 review report by Knudsen and Reading [6], the ECPSSR's account for of the PSS effect has been verified at higher energies, full progress to scrutinize the Coulomb deflection factor and the treatment of the binding effect is important in view of ECPSSR modifications and remains to be made.

2. Modifications of the ECPSSR theory

The ECPSSR goes beyond the first Born approximation which in its standard execution for direct ionization to the target's continuum is the plane-wave Born approximation (PWBA) evaluated with approximate limits for momentum transfers and nonrelativistic screened hydrogenic wavefunctions. The ECPSSR accounts for the energy loss (*E*) and Coulomb deflection (*C*) of the projectile and the perturbed-stationary state (*PSS*) and relativistic (*R*) nature of the target's inner shell. For its ECusPSSR modification, the PSS factor that was derived in the separated atom approach of the ECPSSR is replaced with a united and separated usPSS factor [7]. In the eEusPSShsR modification, the *E* and *R* functions of the ECPSSR theory are obviated by a choice of Hartree–Slater relativistic wavefunctions (hsR) and the momentum transfer limits with exact energy loss (eE) [8]. In the eEqCusPSShsR and eEmCusPSShsR modifications the Coulomb deflection factor *C* of the ECPSSR theory is replaced by factors derived, respectively, quantum-mechanically qC [9] or semiclassically in the monopole approximation mC [10] as evaluated in [11].

3. Verification of the PSS effect with antiproton/proton ratios for H and He ionization

In excellent agreement with the close-coupling (cc) calculations [2,12], Fig. 1(a) shows how the polarization effect of the ECPSSR enhances proton ionization of atomic hydrogen. Fig. 1(b) demonstrates – again in excellent agreement with [12,13] – how the antipolarization effect of the ECPSSR diminishes antiproton ionization of atomic hydrogen. Ignoring the obvious discrepancies with the proton data [14–16] in the 0.001–0.01 MeV regime that is inaccessible to antiprotons, in the 0.01–0.1 MeV range the proton data of Shah et al. [15] as well as the antiproton measurements of Knudsen et al. [17] are overestimated by the ECPSSR and cc calculations [2,12,13]. As seen in Fig. 2, however, the ECPSSR ratios of antiproton-to-proton cross sections are in very good agreement with the antiproton [17]/proton [15] data while the calculations of [2,12,13] give somewhat lower ratios. On the other hand, two-center expansion calculations of Ermolaev [18] and Toshima [19] are in excellent agreement with the proton data [14,15] yielding only slightly larger

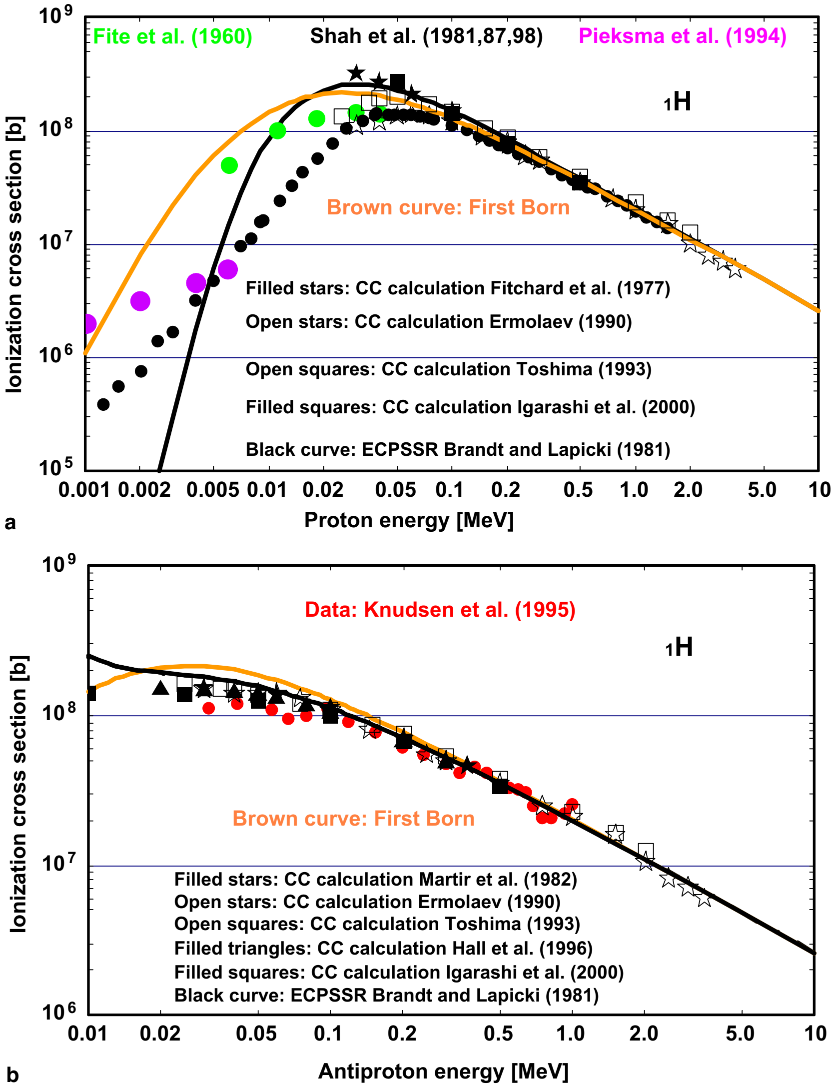

Fig. 1. Ionization of H by protons and antiprotons. Experimental proton (midsize [14], small [15] and large [16] circles) and antiproton (circles [17]) cross sections are compared with the predictions of the first Born (orange) and ECPSSR (black [1]) curves and other theories (filled stars for protons [2], filled stars and triangles for antiprotons [3,13], plus filled squares [12], open stars [18] and squares [19] for proton and antiproton cross section). (For interpretation of the references in color in all figure legend, the reader is referred to the web version of this article.)

ratios than the ECPSSR calculation. It appears that two-center expansions in [18] and [19] are the key to better results – while multi-cut forced impulse method of Reading et al. [20] failed to bring their previous results in line with the antiproton experiment [17] their recent calculation based on a coherent addition of target- and projectile-centered amplitudes for 0.02-MeV protons on H [21] agrees with a fitted value of [22].

It should be noted that relative to [2,12,13] the antiproton data [17] were – within 5% – less overestimated in [23] and [24] while they are more overestimated in other recent theories [25–27] as exhibited in Figs. 1 and 3 of [24]. It is difficult to

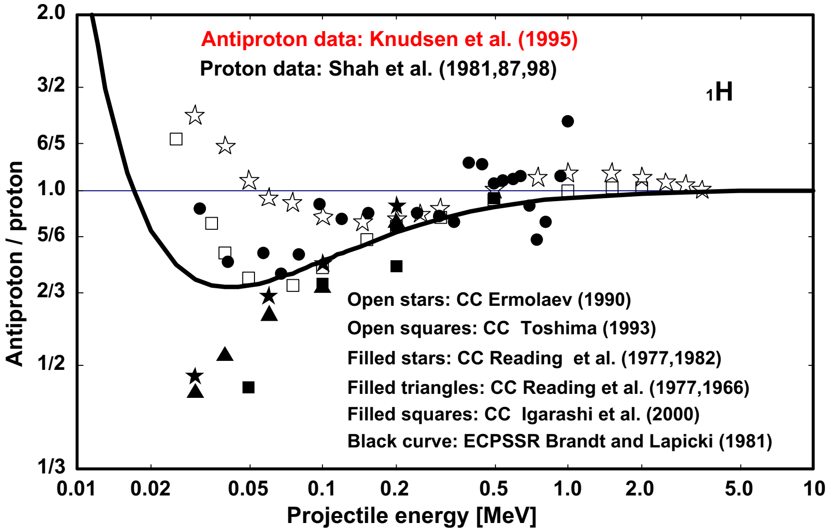

Fig. 2. Antiproton/proton ratio for ionization of H. Experimental ratio of antiproton [17] to proton [15] cross sections (circles) is compared with the predictions of the ECPSSR (curve [1]) and other theories (filled stars [2,3] and triangles [2,13], plus filled squares [12], open stars [18] and squares [19]).

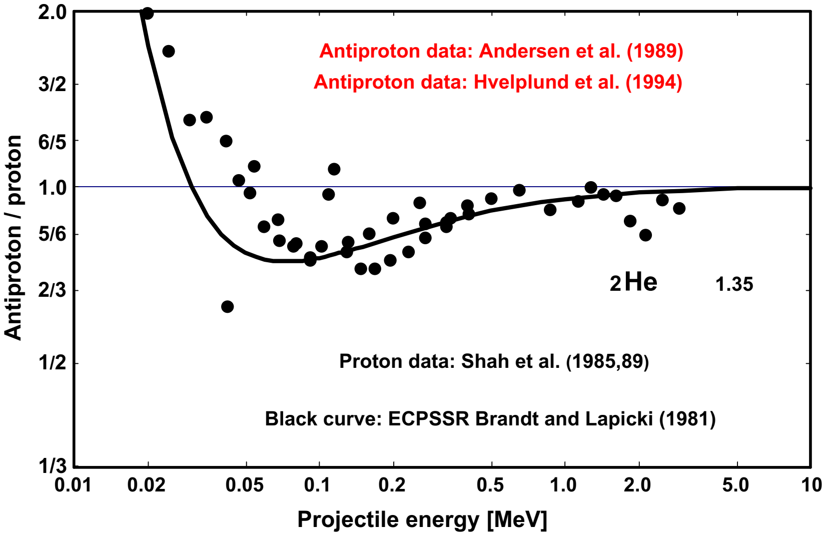

Fig. 3. Antiproton/proton ratio for ionization of He. Experimental ratio of antiproton [38,39] to proton [41] cross sections (circles) is compared with the predictions of the ECPSSR (curve [1]).

deduce what antiproton/proton ratios emerge from [23–27] because there are no results of their particular methods for H ionization by protons. In a stark contrast with the ECPSSR that predicts a continuous increase of the ionization cross section as the antiproton energy decreases, Figs. 1 and 2 in [24] show that even with an account for Coulomb trajectory the ionization cross section gradually decreases from its peak value of 1.5×10^8 b at about 25 keV to 1.2×10^8 b at

0.1 keV. A minimum of 1.3×10^8 b at 2 keV and only a gradual increase to 1.7×10^8 b at 0.2 keV was calculated in [28]. While 0.1 keV would be at the experimental threshold for delivery of ultra slow antiprotons [29], the antiproton measurements [17] terminate prematurely at 0.03 MeV to see the onset and role of the antibinding and the Coulomb deflection effects predicted by the ECPSSR theory for H ionization. As noted by Widmann, down to 0.02 MeV "the various theoretical models agree well with the data, but below they widely disagree. New experimental data for various targets at energies down to 1 keV are therefore urgently needed to distinguish between the theories" [30]. Ionization of H by less then 0.02 MeV protons is equally problematic. Although the proton data [15] have been found in perfect agreement with calculations down to 0.005 MeV [31,32] and even 0.001 MeV [33], the discrepancies of these theories with other data [14,16] and a factor of 9 discrepancy between [14] and [16] at 0.006 MeV (see Fig. 1) might explain why these data or a semiempirical fit of Rudd et al. [22] (not shown here) – that in agreement with [34] tracks these measurements halfway between [15] and [14,16] and converges to the 0.001 MeV datum [16] – would have failed to provide for a definitive experimental test of the ECPSSR theory with the antiproton/proton ratio even after antiprotons will be slowed down to 0.005 MeV at the GSI's future Facility for Low-energy Antiproton and Ion Research (FLAIR) [35].

An antipolarization effect was also noted in He bombarded by 0.5–5 MeV antiprotons [36] – notwithstanding that observed cross sections were 6% higher than in the measurements of [37].

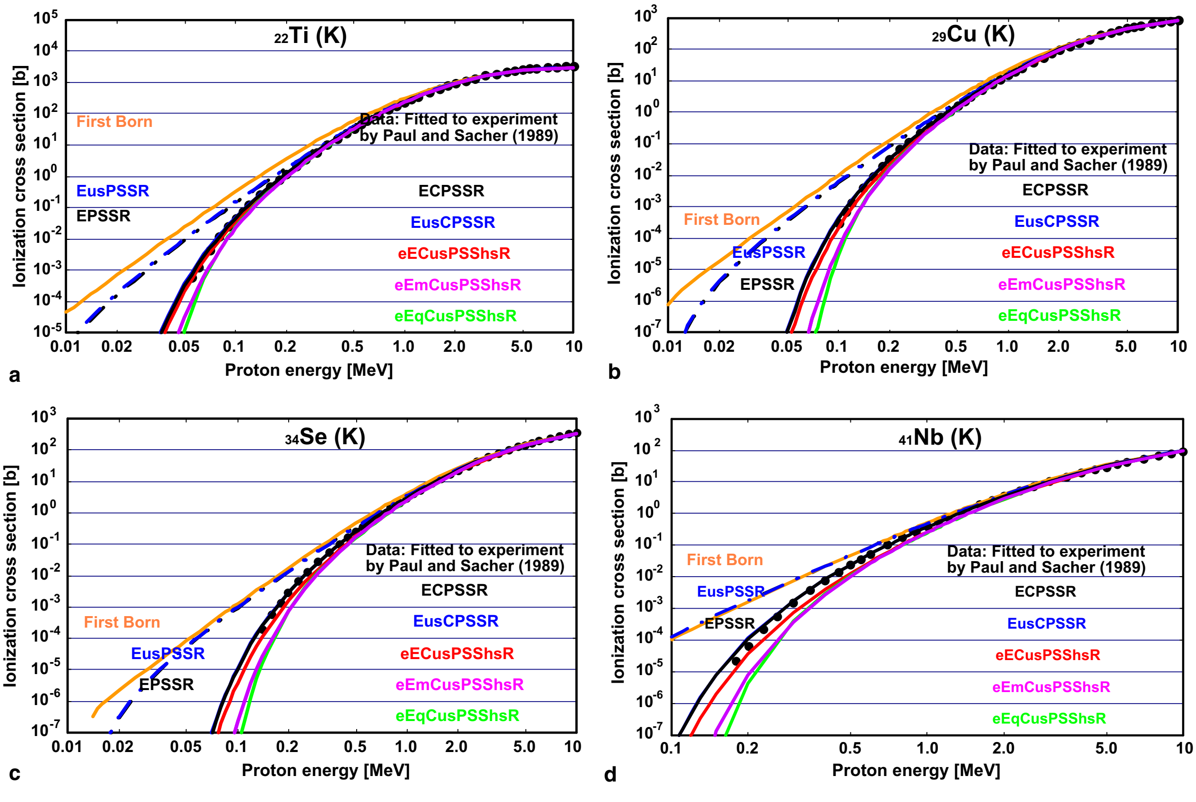

Fig. 4. K-shell ionization of titanium, copper, selenium and niobium by protons. The fitted experimental cross sections (circles [45]) are compared with the predictions of the first Born (orange curve) and ECPSSR (black curve [1] that is the closest to the data) theories and modifications to the ECPSSR theory as labeled and referenced in Section 2.

Clearly demonstrated in the later work of Andersen et al. [38], and continued by Hvelplund et al. [39] down to 0.013 MeV, the antibinding was also confirmed. The measured antiproton/proton ionization ratios in He agree very well with the ECPSSR theory as seen in Fig. 3 as they do identically with the CDW-EIS [40]. Interestingly, the ECPSSR and the CDW-EIS overestimate the proton [41] and antiproton [38,39] data for He by 30% at 0.5 MeV and, in a manner replicating what was seen for hydrogen, progressively more below this energy.

In the ECPSSR calculation that utilizes the screened hydrogenic wavefunctions, the effective Z_2 was set to 1.35 to match the observed binding energy in He. Although the classical-trajectory Monte Carlo calculation shows the antiproton/proton ratio as insensitive to the choice of Z_2 in the limited range of 0.1–5 MeV [42], with Slater's prescription of $Z_2 = 1.7$, the cross section would be too large below the peak and in good agreement above the peak, while with the effective $Z_2 = 1$ the calculated ionization cross sections would agree with the data at low energies but fall unacceptably low above the peak. An energy-dependent effective Z_2 that reflects the critical dynamics of the screening in outer shell electrons would be warranted as it might have been appropriate in calculations of total ionization in Ne, Ar, Kr and Xe for which 0.029–1.1 MeV antiproton data are found in

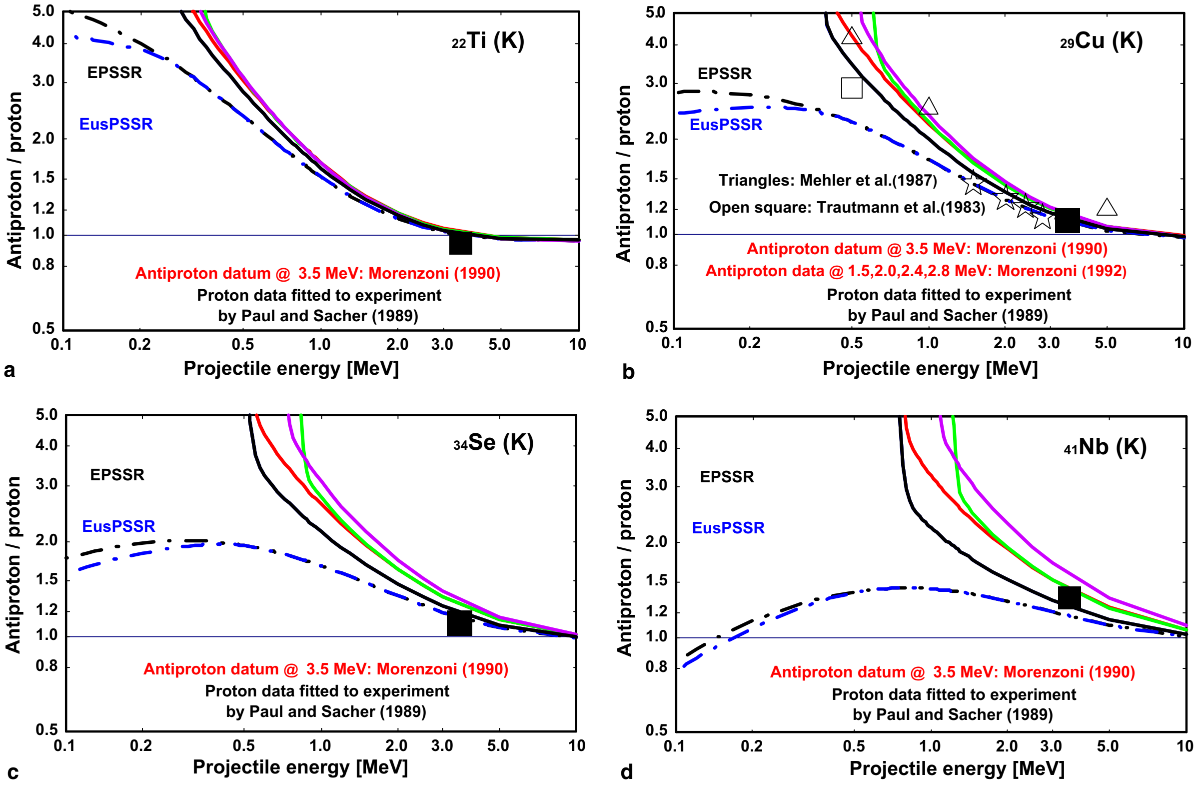

Fig. 5. Antiproton/proton ratio for K-shell ionization of titanium, copper, selenium and niobium. Experimental ratio at 3.5 MeV (square [44]) is at too high energy for differentiation between the predictions of the ECPSSR theory (black curve [1]) and its modifications as labeled and referenced in Section 2. For copper, at 0.5 MeV the ECPSSR prediction falls in between semiclassical result of Trautmann et al. (square [46]) and the cc calculations of Mehler et al. (triangles [47]). Morenzoni's ratios for K-shell ionization of Cu in the 1.5–2.8 MeV range (stars) as displayed in [50] tend to support the ECPSSR theory over its modifications but they were taken at too large energy for a definite conclusion.

Paludan et al. [43]. While the ratios of the antiproton-to-proton cross sections are consistent with the PSS treatment of the binding/polarization effects, the lowest projectile velocities of order of 1 a.u. that are comparable with speeds of electrons in the outer shells are too high to see the difference with the united and separated atom modification of the ECPSSR theory or even begin to note the effect of the Coulomb deflection.

4. Testing the Coulomb deflection effect with antiproton/proton ratios for K-shell ionization

Morenzoni demonstrated the great accuracy of the ECPSSR in the prediction of both antibinding/binding and antipolarization/polarization effects by measuring antiprotons-to-protons ratios of the K-shell ionization cross sections in $_{22}$Ti, $_{29}$Cu, $_{34}$Se and $_{41}$Nb at a single energy of 3.5 MeV [44]. As seen in Fig. 4, the ECPSSR is in excellent agreement with ionization cross sections by 3.5-MeV protons and continues to agree with the fit to the massive data base compiled by Paul and Sacher [45] except at the lowest energies where it systematically and increasingly overestimates the fitted data, and where the modifications of the ECPSSR come to play. For the elements of the Morenzoni measurements, one would have to go down below 0.03 MeV for $_{22}$Ti or 0.3 MeV for $_{41}$Nb to see the need for a modification of the ECPSSR theory. As displayed in Fig. 5, one could start to differentiate between the outcomes of various ECPSSR modifications with antiproton energies below 0.3 MeV for $_{22}$Ti or 3 MeV for $_{41}$Nb, i.e. the energies that are an order of magnitude above where these modifications become important in ionization by protons. Experimental antiproton/proton ratios below these energies would have provided a sharper picture for the distinction and isolation of the optimal choice of the proper Coulomb deflection factor! They would also provide an experimental test of other theories of inner-shell ionization [46–48]. The existing predictions of two them [46,47] for K-shell of copper are clearly different at 0.5 MeV as they would be between [47] and [48] for K-shell ionization of silver at 0.2 MeV and similarly in L-shell ionization of gold [48]. Measuring such ratios at 3 MeV that was proposed as a test of the ECPSSR treatment of the Coulomb deflection and antibinding/binding effects [49] would have been too high energy for this purpose. Morenzoni's ratios for K-shell ionization of Cu at 1.5–2.8 MeV, as communicated in 1992 to Hansteen et al. [50], are still at too large energies for a definitve test of inner-shell ionization theories [1,7–11,46–48].

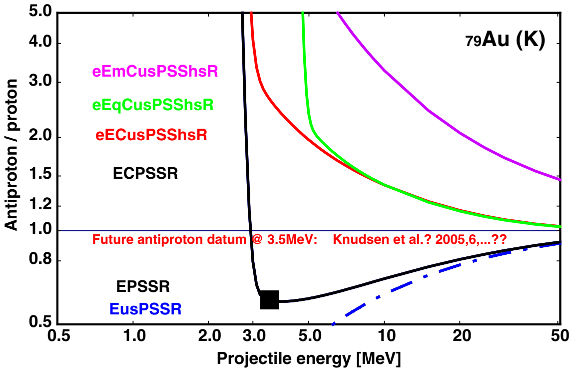

Fig. 6. Antiproton/proton ratio for K-shell ionization of gold according the predictions of the ECPSSR theory (black curve [1]) and its modifications as labeled and referenced in Section 2. A measurement of that ratio at 3.5 MeV would allow for a definitive assessment of the Coulomb deflection as employed in the ECPSSR theory vis a vis its modification and results of other theories. If the yet-to-be-measured K-shell ionization cross section of Au by 3.5-MeV antiprotons was 0.017 b, then its hypothetical ratio to the proton cross section (see square) would be in perfect agreement with the ECPSSR theory.

5. Conclusions

Since the cross section for K-shell ionization of copper by 0.5 MeV antiprotons is 10^7 smaller than for ionization of hydrogen, it would be quite a challenge to measure that cross section although "for beam energies down to 0.5 MeV the [antiproton] momentum resolution is still acceptable for most experiments" and "measurements planned at lower energies should elucidate the role of the Coulomb correction, which is the subject to large uncertainties" [44].

The same goal could be achieved at larger energies with measurements on *heavy* elements. As shown in Fig. 6, in ionization of gold this could have been done with 5.9 MeV antiprotons that were routinely extracted from LEAR. As indicated be a hypothetical data point to be taken in the future, with a slight degradation of the antiproton beam to 3.5 MeV of [44], one would have the optimal energy to elucidate the role of the Coulomb deflection factor, to distinguish between various modifications of the ECPSSR theory, and to set the gold standard for other theories of inner-shell ionization by protons and antiprotons.

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