3.1 Laser Spectroscopy of Antiprotonic Helium Atoms

D. Horváth, B. Juhász, E. Takács (ASACUSA collaboration)

In 2002, laser spectroscopy studies of antiprotonic helium atoms \((\bar{p} - e^- - \text{He}^{++} \equiv \bar{p}\text{He}^+)\) were carried out at the Antiproton Decelerator (AD) of CERN in July and August. The experiments used both the direct AD antiproton beam (energy: 5.3 MeV) and the decelerated beam (energy: 20–120 keV), which were produced using the Radio Frequency Quadrupole Decelerator (RFQD), a unique device which both decelerates and focuses the antiproton beam. Unlike the previous year, this time an S-shaped achromatic spectrometer line was added between the exit of the RFQD and the entrance of our cryostat. This spectrometer line only transports the decelerated antiprotons to the cryostat, while the undecelerated antiprotons (appr. 50% of the beam) annihilate far from the cryostat, thus reducing a major source of background in the annihilation time spectrum.

Another new equipment we started to use was a high-pressure, high-purity target chamber for room temperature measurements. The chamber has one stainless steel window for the antiproton beam, and three quartz windows for the laser beams to allow both traditional collinear single-photon spectroscopy and Doppler-free two-photon spectroscopy. This chamber can be used with the direct 5.3-MeV antiproton beam.

Using the old and new equipment, the following experiments have been made:

High-precision measurements of the wavelengths of transitions between five pairs of metastable and short-lived antiprotonic states in low-density (0.1–5 mbar) \(^4\text{He}\) and \(^3\text{He}\) [1]. Using the above-mentioned achromatic spectrometer line to increase the signal-to-noise ratio, the precision of the measured transition wavelengths will likely to increase, which in turn can improve our previously obtained precision of the mass and charge of the antiproton, a test of the CPT invariance [2,3].

The above-mentioned measurements at low densities (<1 mbar) revealed that the average lifetime of antiprotons (which can be deduced from the average decay rate of the delayed annihilation time spectra) increases to \(~5\) microseconds compared to 3.5 microseconds at higher densities (>100 mbar) [4]. This reflects the reduced collisional influence at such low densities.

We also found that at even lower densities (<0.1 mbar), the decay lifetime of the laser-induced annihilation spike becomes significantly longer (\(~10\) ns vs. \(~\text{ns}\) [4]. This indicates that the \(\bar{p} - \text{He}^{++} \equiv \bar{p}\text{He}^{++}\) ion, which is created after the Auger transition from the daughter state of the laser-induced transition, has a longer lifetime due to a reduction of the collisional Stark mixing in such ultra-low density environments.

Discovery of four new laser resonant transitions between antiprotonic states, one in \(^4\text{He}\) and three in \(^3\text{He}\) [4]. The wavelengths of these transitions were also measured. A high-resolution scan of one of the transitions revealed a double peak, which is caused by the hyperfine splitting of the parent and daughter states (see Fig. 1).

![Figure 1. High-resolution scan of a resonance transition with a doublet splitting.](image-url)
ening, which can be eliminated using Doppler-free two-photon laser spectroscopy technique. The feasibility of this method was tested in 2002 using the high-pressure target chamber and two collinear laser beams. The measurements had to be made at room temperature, where Doppler broadening is larger than the laser bandwidth so that we can see a narrowing of the resonance line due to Doppler cancelling. The transition was successfully observed, but the measured linewidth was much larger and the signal-to-noise ratio was much smaller than those of the single-photon transitions. The possible reasons for the poor experimental results can be the increased i) collisional broadening, ii) laser bandwidth, iii) laser wavelength and power fluctuations.

Investigation of the temperature dependence of quenching of metastable states in collisions with H$_2$ and D$_2$ molecules [5]. According to the theoretical calculations of Sauge and Valiron [6], a state-dependent activation barrier exists for this kind of quenching reaction, which means that the quenching cross section $\sigma_q$ should increase with increasing temperature following the Arrhenius law:

$$\sigma_q = \sigma_0 \exp(-E_b/kT),$$

where $\sigma_0$ is the cross section at infinitely high temperatures (this we expect to be close to the geometrical cross section), $E_b$ is the height of the activation barrier, $k$ is the Boltzmann constant and $T$ is the temperature. However, all previous measurements of quenching by hydrogen and deuterium molecules were done at 30 K [7]; therefore, in order to test the above temperature dependence, we made measurements at several temperatures: at room temperature using the high-pressure target chamber and at 25–100 K using our usual high-density cryostat, and we found that indeed there is a significant temperature dependence. In case of one antiprotonic state, we could systematically study this dependence by measuring the quenching cross section with deuterium at six temperatures. The collected data, however, favour a different model:

$$\sigma_q = \sigma_0 \exp(-E_b/kT) + \sigma_c,$$

where $\sigma_c$ is independent of the temperature. This term is most likely related to the quantum tunnelling of the colliding impurity molecule through the activation barrier. Fig. 2 shows the quenching cross section versus the inverse temperature. A deviation from the Arrhenius law is clearly visible (note the logarithmic scale of the vertical axis). The plotted line is the result of fitting Eq. (2) to the data points.

![Figure 2. Quenching cross section versus the inverse temperature.](image)

The analysis of the data collected in 2000 and 2001 was partially completed and the results were published [7-10].

Almost all of the support structures of the experimental devices were designed and manufactured in Hungary.

3.2 An improved description of the multiple ionization \(K\beta L^i\) satellite energy spacings

I. Török, T. Papp, S. Raman

In analytical works, and in basic atomic physics research one needs the data of the satellite lines, therefore we began to make a new compilation of the energy shifts of the \(K\alpha L^i M^n N^m \ldots\), \(K\beta L^i M^n N^m \ldots\) satellites, and \(K^2\alpha L^i M^n N^m \ldots\), \(K^2\beta L^i M^n N^m \ldots\) hypersatellites. A byproduct of this compilation is a test of the “classic” description of their energy spacings as a function of \(Z\) [1]. The larger database we have now, made it possible, to obtain a better description. For \(K\alpha L^i\) satellites see Ref. [2]. The old version gave equidistant spacing also for the \(K\beta L^i\) satellites, using an average effective \(Z\) seen by the electrons: 
\[
\Delta E(K\beta L) = 4.38 Z_L = 4.38(Z - 4.15),
\]
our version uses an effective \(Z\) changing with the number of spectator L vacancies:
\[
\Delta E(K\beta L^i) = i \times 3.37[Z + (i - 1) \times 0.5 - 5.37]
\]
\(i = 1, 2, 3, \ldots, 7\)

This equation, obtained by fitting a representative portion of our compiled data is in agreement with experimental data, perhaps the \(i = 7\) case is a little bit underestimating them, probably because of the significant number of additional M, N vacancies. Full account is given in a paper in preparation.

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3.3 On the measurements of $K^2\beta L^i$ hypersatellites

I. Török

Although we gave a short publication in our institute’s Ann. Rep., there was stated in the literature, that such new formulae for the $K\beta L^i$, and $K^2\beta L^i$ satellites and hypersatellites are not existing. In [1] we gave a semiempirical formula for the $K\alpha L^i$ satellite energies, and in [2] for the $K\beta L^i$ lines, this latter report we republish in this Ann. Rep., with the original title, containing the symbol $\beta$ (which was lost during the editorial process in the case of first publication), emphasising the new content. Regarding the $K^2\beta L^i$ hypersatellites they were not measured at all by crystal spectrometers.

The $K^2\beta L^i$ hypersatellites are very weak lines. They are regarded, as not available for measurements by crystal spectrometers. Nowadays the situation is changing, the better and better resolution and the use of high efficiency position sensitive detectors makes these hypersatellites to become investigable. In a pair of spectra (Ca and Ti) - I got from the authors (the group of prof. J.-Cl. Dousse) prior to publication [3], - there were a few weak, but definite, although unassigned lines, which comparing to our multiple ionization satellite energy systematics [2], turned to be such hypersatellites, including their $K^2\beta L^i$ satellites. We found also an indication of such hypersatellites for Ti in the literature [4], dated about ten years earlier. The Dousse-group was informed about our observation in their spectra, and as to my knowledge, now a project is running successfully to measure such hypersatellites in the range of elements around Cr.


3.4 Electron emission from $\text{H}_2^0$ in collisions with He atoms

L. Sarkadi, L. Lugosi, B. Paripás\textsuperscript{a}) and B. Palásthy\textsuperscript{a})

The electron emission in energetic ion-atom (atom-atom) collisions has been widely studied in the past decades, and now it is well understood theoretically. At the same time, the information for the electron emission in collisions involving molecules is rather scarce.

In the present work we studied the electron ejection from the neutral $\text{H}_2$ molecule in collisions with He atoms at impact energy 150 keV amu\textsuperscript{-1}. The work was motivated by a recent experiment [1] in which evidence was found for the coherent electron emission from the two H atoms of the $\text{H}_2$ molecule collided with 60 MeV amu\textsuperscript{-1} $\text{Kr}^{34+}$ ions.

Our measurements were performed at the 1.5 MV Van de Graaff accelerator of ATOMKI. We produced neutral $\text{H}_2$ beam by charge exchange of the $\text{H}_2^+$ beam of the accelerator with the residual gas of the beam channel. For normalization we used a $\text{H}_2^0$ beam of the same velocity. We measured the energy spectra of the ejected electrons at 0\textdegree. The electron emission from $\text{H}_2^0$ and $\text{H}_2^0$ was indentified by detecting the electrons in coincidence with the outgoing $\text{H}_2^+$ and $\text{H}^+$ ions, respectively. The spectra were taken in the cusp region, i.e., we measured the distributions of those electrons which were ejected with small relative kinetic energy with respect to the projectile. The cusp electron production associated with projectile ionization is called electron loss to the continuum (ELC). It was an interesting question whether ELC is affected by any interference effect for molecule projectile.

The obtained electron spectra are displayed in Fig. 1. Surprisingly, the width of the ELC peak for the molecular emission is considerably smaller than that for the atomic emission. The ratio of the corresponding cross sections exhibits a pronounced, narrow peak centered at the cusp maximum.

We applied the classical trajectory Monte Carlo (CTMC) method to the description of the ELC process in collisions of $\text{H}_2^0$ and $\text{H}_2^0$ with He. The coherent electron emission from $\text{H}_2^0$ was treated as it is proposed in Ref. [2]. CTMC predicts a weak dependence of the molecule/atom cross section ratio on the electron energy, in a strong disagreement with the experiment.

Figure 1. Upper part: Measured relative double differential cross sections (DDCS) for the ELC cusp produced in $\text{H}_2^0$ + He (open circles) and $\text{H}_2^0$ + He (full circles) collisions. Lower part: Ratio of the measured and calculated DDCS values as a function of the electron energy. The notations: –o–, experiment; —, CTMC theory. The experimental data are normalized to the theoretical curve at 150 eV electron energy.

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3.5 Strong nondipole effect in 5s photoionization of xenon

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Dipole approximation has often been used successfully to describe the angular distribution of photoelectrons and also to evaluate the experimental angular distribution results. The validity of the dipole approximation comes from the dominance of the dipole interaction at low photon energies ($h\nu \leq 5$ keV). Until recently the contribution of the higher order multipole components were assumed to be negligible.

Intensive theoretical investigations related to nondipole effects at low photon energies began during the last decade. Recent experimental investigations of the photoionization angular distribution \cite{1}\cite{2}, extending down to 250 eV photon energies, suggested that nondipole effects are of importance at low photon energies.

In present work, the angular distribution of the 5s photoelectrons of xenon was measured with linearly polarized light in the 90-225 eV photon energy range in order to determine the dipole ($\beta$) and nondipole ($\delta$ and $\gamma$) parameters. The measurements were carried out at the beam line I411 on the third generation MAX-II storage ring in the Max-Lab, in Lund, Sweden \cite{3}\cite{4}. Emitted electrons were detected by 20 channeltrons using ESA-22 electron spectrometer \cite{5}, which was installed before the permanent end-station into so called one-meter section. For present measurements the relative energy resolution of the analyzer was set to $\Delta E/E = 2.4 \times 10^{-3}$. This resolution and the bandwidth of the photon beam (bandwidth using 120$\mu$m exit slit varied between 0.09 and 0.3 eV depending on incident photon energy) ensured that the Xe 5s photoline could be separated from the closest satellite line.

The correct intensity calibration the relative efficiencies of the detectors were determined by using isotropic Ar $L_2 - M_{2,3}M_{2,3} \, ^3P_{0,1,2}$ Auger transitions.

The angular anisotropy parameters were extracted from the experimental, efficiency corrected intensities using equation \cite{6}

$$
\frac{d\sigma_{nl}}{d\Omega} = \frac{\sigma_{nl}}{4\pi} \left\{ 1 + \beta P_2(\cos \theta) + [\delta + \gamma \cos^2(\theta)] \cos(\phi) \sin(\theta) \right\}
$$

that describes angular distribution of photoelectrons for linearly polarized light. $P_2$ is the second order Legendre polynomial, $\sigma_{nl}$ is the photoionization cross section of the $nl$ orbital, $\beta$ is the anisotropy parameter of the dipole interaction (E1), $\delta$ and $\gamma$ are the parameters related to the quadrupole interaction (E2), whereas $\theta$ and $\phi$ define the polar and azimuthal angles relative to the polarization vector, respectively.

![Figure 1. Comparison of the experimental nondipole $\gamma$ parameters (open circles) with the corresponding theoretical values as a function of the photon energy. Theory: RIPM \cite{8} (dot line), 13-channel RPAE \cite{11} (dash-dot-dot line), 13-channel (dash line) and 20-channel RRPA (solid line) \cite{9}](image)

The dipole and nondipole parameters were obtained by the least squares fitting procedure to Eq. (1). Due to used geometry the $\delta$ and $\gamma$ parameters could be determined separately, however, the $\delta$ parameter was found to
be very close to zero as expected theoretically (see e.g. [6] and references therein). The value of the fitted $\beta$ and $\gamma$ parameters did not change practically either the $\delta$-parameter was included or not. Figure 1. compares our experimental and theoretical [8][9][12] nondipole $\gamma$ parameters. The RIPM approximation [8] shows slightly increasing line without any structure, while the $\gamma$ parameter values calculated with 13 or 20-channel RRPA [9] show an enhancement with maximum around 160 eV. Our experiment shows similar structure than these theoretical predictions. The shape of the experimental cusp is similar to the 20-channel calculation but the maximum of the experimental values is smaller. Comparison between theoretical [8][9][12] and present experimental values shows that the inclusion of the Xe 4s and 4p channels is important in the description of the energy dependence of the $\gamma$ parameter in 5s ionization. The contribution created by the 4p channel is, however, slightly overestimated [9]. This is not surprising as the Xe 4p$^{-1}$ is known to correlate with 4d$^{-2}$nf, $\epsilon$f states and this correlation is not included in the calculations.

Amusia et al [12] presented theoretical values for $\gamma$ parameter in Xe 5s photoionization. Their RPA calculations with exchange (RPAE) included coupling between 4d, 5s and 5p channels. The values are smaller over the whole energy range of interest than the corresponding values of Johnson and Cheng [9] indicating that relativistic effects are of some importance.

Remaining discrepancies between experiment and theory may be related to the omission of the satellite channels of the type 5p$^{-2}$nd, ed and 4d$^{-1}$nf, $\epsilon$f related to the 5s and 4p ionizations, respectively, in the calculations.

Figure 2. compares the present and the previous [7] experimental $\beta$ parameters and the corresponding theoretical values [9][10] in the 90-220 eV photon energy range. The results of the relativistic independent particle approximation (RIPA) [8], which omits the coupling between the continuum channels, do not show any sudden changes and $\beta$ has a constant value of about 2. However, all calculations which take the channel interaction into account predict a broad minimum around 150 eV photon energy. The minimum is deeper in 13-channel than in 20-channel RRPA calculation [9]. The depth further decreases in predictions based on the relativistic time-dependent density functional theory (TDDFT) [10], which include also the correlation related to satellite channels in an average way by a model potential. The present experimentally determined $\beta$ parameters are between 20-channel RRPA and TDDFT values, slightly closer to the results of the 20-channel RRPA calculations. This indicates that the influence of the 4p channel is important in the Xe 5s ionization but that the TDDFT fails in accounting the additional correlation correctly. In general, experimental $\beta$ parameters agree well with theoretical ones [9] except in the 90-130 eV photon energy range where experimental and theoretical values deviate significantly (∼10%).
beta values show narrower and shallower dip than ours or the calculated ones [9]. Furthermore the position of the minimum is shifted to lower photon energies. The difference between the two experimental results requires further investigations.

The effects of the nondipole interaction are remarkable over a wide photon energy range. Especially, at 155 eV photon energy, where the parameter reaches its maximum, the nondipole contribution to total angular distribution is as high as 20%. It is clearly enough to question the validity of the dipole approximation in photoionization of the Xe 5s subshell relative far from the ionization threshold.

Acknowledgements

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3.6 X-ray imaging of ECRIS plasmas

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Introduction

Highly charged ion plasmas generated in the ATOMKI ECR ion source had been imaged using an X-ray CCD device of the National Institute of Standards and Technology (NIST). The motivations for the experiments came from possible future high-resolution X-ray spectroscopic measurements using X-ray microcalorimeters and crystal spectrometers. In the present set of experiments, the general distribution of the emitting highly charged ion cloud and its systematic dependence on various operating parameters were the focus of our interest. Understanding the details of the ion production and confinement provides insight into the operation of the ECR ion source and gives important information for our future spectroscopic plans. In addition to its source diagnostic value, the X-ray imaging and spectroscopy of highly charged ion plasmas can also be utilized for the laboratory investigation of plasmas of astrophysical and other interests.

X-ray imaging

The NIST CCD camera used in these experiments has 1152x1242 pixels in a rectangular arrangement. The imaging was achieved using an appropriately positioned 70 micrometer diameter X-ray pinhole. The CCD chip was thermoelectrically cooled to about $-45^\circ$C to reduce thermal noise. Each pixel can be used in single photon detection mode with an energy resolution of about 180 eV. This feature allows the post detection filtering of the obtained images according to the wavelength of the detected X-ray photons. This can be used to discriminate certain characteristic line emission features in the spectra to determine their distribution in the plasma [1]. The data acquisition and analysis system was partly developed by us using the ROOT data analysis library.

ECR plasmas

For our imaging studies, we have operated the ECR under different running conditions in order to better understand the dynamics of the ion generation. We used working gases of Ar, Xe, O\textsubscript{2}, and solid ferrocene (an organic compound containing Fe). In order to have a clear view of the source the injection side end cap of the plasma chamber has been modified. The pinhole was mounted 91 cm from the center of the plasma and the pinhole – CCD distance was 25 cm forming an X-ray camera with demagnification of 3.6. This permitted more than half of the plasma volume to be imaged through a course mesh; considered to be sufficient because of the 120 degree symmetry of the ECRIS.

![Image generated by an Ar plasma in the ATOMKI ECRIS.](image)

Systematic studies

In these first sets of imaging measurements, the basic features of the ECR plasma X-ray emission were studied under different running conditions. An image generated by an Ar plasma is shown in Figure 1. The upper part of the source is vignetted by a horizontal cut due to the design of the injection side end cap. The two arms showing strong emission

Figure 1. Image generated by an Ar plasma in the ATOMKI ECRIS.
are mainly due to bremsstrahlung and characteristic X-rays generated by high-energy electrons impinging onto the opposite side end cap. The circular aperture of the extraction hole is clearly visible in the center. In a completely different process the more or less circular plasma cloud emits characteristic radiation of the Ar working gas caused by core vacancy creation due to electron impact. An interesting feature is the upside down triangle showing reduced intensity emission, which we tentatively attribute to X-ray absorption within

Figure 2. X-ray spectra from different parts of Figure 1.

Several sets of images similar to Figure 1 have been taken under different running conditions in order to study the origin of the different features in the pictures. These include running the ECRIS in low and high power modes, at different magnetic field settings, and turning the ion extraction on and off etc. We took pictures of mixed plasmas (Ar + Xe, Ar + O2) as well. In addition to the images that have several X-ray photons hitting a single pixel during the exposure, we have also taken low light level images. In these cases, the collected charge in a single CCD pixel is proportional to the energy of the detected X-ray photon, therefore, under these conditions spectral analysis of the X-rays is also possible. As an example Figure 2 shows two of such spectra obtained under the same running conditions as Figure 1. The spectra are from two different regions of the image, the upper corresponding to one of the bright arms and the lower to a region of the Ar plasma cloud. The difference in the strength of the different characteristic emission lines is clearly visible indicating the size and distribution of the plasma (Ar emission) as contrasted with the Al emission from electrons striking the end walls of the plasma chamber. The analysis of the large amounts of data and model calculations are under way.

Conclusions

X-ray images taken under different ECRIS running conditions reveal the hottest, most energetic regions of the plasma. Spectral filtering allows us to study the origin of certain spectral features (e.g. characteristic lines, bremsstrahlung continuum) in the plasma, which can help to improve modeling of the source and other magnetically confined plasmas.

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3.7 Cascade transition x-rays from electron capture into highly charged ions in collisions with neutral gas targets

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In collisions of low energy (few keV/u), highly charged ions (HCIs) with neutral atoms, the electron capture process is far dominant over other processes such as excitation or ionization. It is well established that an electron from a target atom is usually captured into high a Rydberg state of the projectile ion \cite{1}. Even in multi-electron target atoms, single electron capture is generally dominant, though the contribution of double and triple electron capture becomes significant for higher ion charge states. In the case of multiple electron capture, Auger electron emission becomes an important first step of the relaxation process \cite{2}. In essentially all cases (single or multiple capture), however, the stabilization ends in a cascade of photon emitting transitions. When the projectiles are highly charged, the photons emitted in these final steps are x-rays. The observation of these x-rays can provide information on both the electron capture and the following cascade. Recently, the unexpected observation of x-rays from comets and other objects of the solar system \cite{3} brought the collisions of highly ionized projectiles with neutral gases into the forefront of research.

Using the electron beam ion trap (EBIT) \cite{4} and extraction facility \cite{5} at the National Institute of Standards and Technology (NIST), we have performed a series of systematic collision studies with different projectile and target combinations. X-rays originating from a series of the cascades after electron capture into highly excited Rydberg states have been observed from low energy, highly charged Kr\textsuperscript{q+} ions (q=27-36) colliding with neutral Ar atoms. We found that the intensity ratio between L (n=32) x-rays and the sum of M x-rays (n=43, n=53, n=63 etc.) is drastically changed from Kr\textsuperscript{27+} to Kr\textsuperscript{28+} and constant for higher ion charge states (q=29-36). This feature can be understood to be due to the metastable states formed during cascades after electron capture into Kr\textsuperscript{27+}. This is also supported by time-dependent population calculations.

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\textsuperscript{b)} Debrecen University, Debrecen, Bem t 18/a H-4026

\cite{1} R.K. Janev, L.P Presnyakov, and V.P. Shevelko, Physics of Highly Charged Ions (Springer, 1985)
3.8 Double 1s ionization of Mg and Si induced in collisions with fast heavy ions

M. Kobal a, M. Kavčič a, M. Budnar a, J.-Cl. Dousse b and K. Tőkési

The Kα x-ray emission spectra of Mg and Si excited with 34 MeV C ions and 50 MeV Ne ions have been measured with a von Hamos crystal spectrometer [1]. The energy resolution of approximately 0.5 eV was achieved enabling us to distinguish contributions originating from states with different number of holes in K and L shells. In order to determine the intensity of the hypersatellite and satellite lines the model spectra based on the MCDF calculations was constructed and fitted to the measured spectra. The intensities of the measured hypersatellite and satellite lines were used to determine the yield of the KXLN vacancy states produced in the collision, taking into account whole decay scheme of the particular initial KXLN ionized state. The decay scheme has been calculated using the initial rates of the radiative and nonradiative transitions from [2, 3] which were then corrected for additional vacancies in the inner shell according to statistical approach, first proposed by Larkins [4].

From the yield of the doubly 1s ionized states (K2XLN) produced in the collisions relative to the singly 1s ionized states (K1LN) the ratio of double to single 1s ionization cross section has been obtained. The double to single 1s ionization cross section has been also calculated in the independent electron model using the one electron ionization probabilities calculated within the three body classical trajectory Monte-Carlo simulation (CTMC). The calculated values are presented in Table 1. In such nearly symmetric collisions electron capture by the projectile is actually the dominant ionization mechanism. Since the capture in the 1s shell of the projectile is by far the strongest the ionization cross section depend significantly on the charge of the projectile. In Table 1 we can find the calculated values for the projectile with 0, 1, 2 electrons in its K shell and for the projectile with the average equilibrium charge in the solid target used in our experiment.

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We found, except for the case of 34 MeV C6+ → Mg collision, a relatively good agreement between the experimental and calculated data.

a) Jožef Stefan Institute, Ljubljana
b) Physics Department, University of Fribourg

3.9 Fermi-shuttle acceleration in low and intermediate velocity ion-atom collisions

B. Sulik\textsuperscript{a)}, R. Hellhammer\textsuperscript{b)}, Z.D. Pešić\textsuperscript{b)} and N. Stolterfoht\textsuperscript{b)}

We have been performing a systematic search for accelerating multiple scattering sequences of electrons emitted in ion-atom collisions (or Fermi-shuttle type ionization \cite{Fermi}). In this process, the liberated electron is repeatedly backscattered by the projectile and the target center (denoted by P and T respectively). With the impact velocity of the projectile V, scattering sequences starting with target ionization produce electrons emitted with the mean velocity $2nV$ in both forward and backward directions, where $n$ is the number of encounters with the projectile. Starting with projectile ionization, the corresponding mean velocity is $(2n+1)V$.

In a recent work \cite{Sulik02}, experimental evidence has been found for consecutive P-T-P (projectile-target-projectile) and P-T-P-T ping-pong-like scattering of ionized target electrons in single C\textsuperscript{+} + Xe collisions at 150 and 233 keV/u impact energies. Distinct signatures for triple and quadruple electron scattering have been separated. Typical signature was the excess electron intensity emitted forward and backward in the expected velocity regions.

In the present work, we search for longer sequences in a significantly lower impact velocity range. In an earlier experimental study \cite{Stolterfoht79}, distinct structures of excess electron yields at forward and backward directions have been observed in collisions of 50-400 keV O\textsuperscript{+} ions with Ar target. These structures appeared to be shifted with the projectile velocity \cite{Stolterfoht79}. In our present experiments, performed at the beamline of the ECR ion source of the Ionen-Strahl Labor (ISL) in Hahn-Meitner Institute Berlin, we studied the spectra of electrons emitted in collisions of 15 keV N\textsuperscript{+} ions with Ar atoms under single collision condition. At this low velocity, we enter the impact energy range, where the accelerating electron “orbits” may be considered as specific molecular orbitals, and the Fermi-shuttle process might be treated as a promotion mechanism \cite{Ovchinnikov99}. Our preliminary results show a a significant forward-backward enhancement in the yield of continuous electrons in the 20-100 eV energy range, indicating the presence of 6-12-fold accelerating multiple scattering in the collisions (Fig. 1). Further experimental and theoretical work is needed to confirm these findings.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure.png}
\caption{Double differential cross sections for electron emission in 15 keV N\textsuperscript{+} + Ar collisions, normalized to the Ar LMM Auger group. Multiples of the projectile velocity are indicated.}
\end{figure}

\textbf{Acknowledgements}

We acknowledge support from the OTKA Grant No. T032942, and the Hungarian-German Intergovernmental S&T Collaboration No. D17/99.

a) A significant part of the work was performed during a guest-scientist period in Hahn- Meitner Institute, Berlin.

b) Hahn-Meitner Institute, Glienickerstr. 100, D-14109 Berlin, Germany

3.10 Electron emission from collisions of H$_2^+$ molecule ions with inert gas targets: Search for interference patterns

B. Sulik, T. Ricsóka, O. Turák and N. Stolterfoht$^a$)

In recent years, particular attention has been devoted to charged particle induced ionization of the H$_2$ molecule. Since the two atomic centers in this simple molecule can not be distinguished, their electron emission contributions add coherently. First experimental evidence for such interference effects has been found in the electron emission spectra in collisions of very fast and highly charged (60 MeV/u Kr$^{34+}$) projectiles with H$_2$ molecules [1]. In subsequent theoretical studies [2,3], the basic features have been analyzed. In a recent experimental study, some of their prediction has been verified [4].

The simplest molecular system, however, is not H$_2$ with two electrons, but the H$_2^+$ molecular ion. At first sight, the symmetries of the H$_2$ molecule are also present in this one-electron system, but electron-electron interactions do not alter the picture.

In the present work, we studied electron emission from H$_2^+$ molecule ions colliding with He and Ar targets (the inverse collision system). A beam of 1.5 MeV/u H$_2^+$ ions was directed to gas jet targets, and electron spectra were collected in the entire 0-180° angular range. The experiments have been performed at the beamline of a 5 MV Van de Graaff accelerator at ATOMKI, Debrecen. For reference purposes, we also collected spectra in collisions of 1.5 MeV H$^0$ atoms with the same targets.

In Ref. [2], interference was treated within a two-effective center approximation, which partially accounts the correlation between the emitted and bound electrons. It is not clear, whether interference is only due to symmetry properties, or electron correlation in H$_2$ also plays a significant role.

Our present experiments are expected to answer this question too. We have found clear differences between atomic (H$^0$) and molecular (H$_2^+$) bombardment with the same impact velocity. Preliminary results are shown in Figure 1, comparing the cross sections for H$^0$ and H$_2^+$ impact at 165°. Beyond the shape-difference, a crossing point exhibits at 1140 eV, indicating the presence of interference effects. The oscillation frequency seems to be doubled compared to first order expectations [1,2]. This is in agreement with the picture that electron loss at backward angles is due to hard collisions. Our data also resemble a recent observation of double frequency components for H$_2$ [5]. Further analysis is in progress.

![Figure 1. Double differential electron emission cross sections at 165° observation angle in collisions of H atoms and H$_2^+$ molecules with Ar.](image)

Acknowledgements
We acknowledge support from the Hungarian OTKA Grant No. T032942, and the Hungarian-German Intergovernmental S&T Collaboration No. D17/99.

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3.11 Cascade feeding of the 1s2s2p^4P state in collisions of Li-like O^{5+} ions with H_2 and He targets

B. Sulik, A. Orbán, L. Gulyás and T.J.M. Zouros\textsuperscript{a)}

In the collisional formation of the 1s2s2p^4P state of Li-like ions, one of the possible mechanisms is the so-called transfer-loss (TL) process, in which the loss (ionisation) of a projectile 1s electron occurs simultaneously with the transfer of a target 1s electron to the projectile 2p subshell. This process was studied experimentally in 0.2-2 MeV/u collisions of O^{5+} ions with H_2 and He targets \cite{1}:

\[ \text{O}^{5+}(1s^22s) + \text{He} \rightarrow \text{O}^{5+}(1s2s2p^4P) + \text{He}^+ + e^- . \]

In our earlier analysis \cite{2} we have shown that the TL process could be described qualitatively, within the framework of the independent particle model (IPM). In the present work, we show that inclusion of capture to higher \( n \) shells of the projectile provides significantly improved agreement with experiment. The basic idea is that practically all capture into higher-lying \( n > 2 \) quartet states decay radiatively very quickly to the 1s2s2p^4P state. These photon cascades become increasingly more likely than autoionization with increasing \( n \). Due to the strongly different decay rates, the metastable 1s2s2p^4P state behaves like a quasi-ground state, collecting all quartet capture events before decaying itself.

Compared to our earlier study \cite{2}, only the transfer probability was calculated differently:

\[ P_T^{2\text{pm}} = P_{He(1s) - O(2p)} + P_{He(1s) - O(n>2)} \]

where the first term is the probability of the capture of a He 1s electron to the O^5+ 2p state by a He or H_2 1s electron (original term from our earlier work \cite{2}), and the second term represents capture to all O^5+ + \( n > 2 \) shells.

Similarly to our previous work \cite{2}, calculations of projectile excitation and ionization probabilities were performed by an SCA code \cite{3}, while electron transfer probabilities were calculated in the CDW approximation \cite{4}.

In Fig. 1, experimental data for the O^5+ + H_2 collision system \cite{1} are compared with our present (denoted by ”cascade TL + T^2L”) and earlier calculations (TL + T^2L). It is clearly seen, that the inclusion of the cascade feeding into the calculations significantly improved the agreement with experiment.

Figure 1. Single differential cross sections for zero-degree Auger electron emission from the 1s2s2p^4P state as a function of projectile energy for collisions with H_2. The symbols are for experimental data \cite{1}. The dotted line represents the earlier TL calculations without cascade feeding, while the solid line is the present full TL calculation. The dashed line is a calculation for the dielectronic excitation (eeE) within the electron scattering model \cite{1}.

Acknowledgements

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3.12 Guided transmission of 3 keV Ne\textsuperscript{7+} ions through nanocapillaries in PET polymers: dependence on the capillary diameter

N. Stolterfoht\textsuperscript{a)}, R. Hellhammer\textsuperscript{a)}, Z.D. Pešić\textsuperscript{a)}, V. Hoffmann\textsuperscript{a)}, S. Petrov\textsuperscript{a)}, D. Fink\textsuperscript{a)}, B. Sulik\textsuperscript{b)}

The outstanding progress in nanotechnology is accompanied by a continuous miniaturization of interfaces used in microelectronics and related fields. Particular attention has been paid to linear structures of mesoscopic dimensions, such as pores or capillaries. Recently, we started experiments in which PET (Mylar) polymer foils of 10 nm thickness were irradiated by 400 MeV xenon. Capillaries with a diameter of a few hundreds nm in foil were obtained etching ion tracks using NaOH \cite{1}.

To study the capillary interior, we measured the transmission of 3 keV Ne\textsuperscript{7+} ions through capillaries. Foils with different capillary diameters (100 nm \cite{1}, and 200 nm) were tilted with respect to the incident beam direction. Angular distributions of the transmitted Ne\textsuperscript{7+} ions obtained with PET material were found to be essentially different from the results with capillaries covered by a thin Ag metal film. For the latter case, the Ne\textsuperscript{7+} angular distribution is rather narrow (FWHM of 10\(^\circ\)) and ion transmission vanishes when the foil is tilted (Fig. 1). On the contrary, for the 50\(^\circ\) tilted isolating PET foil only about 20\% of the angular distribution of the Ne\textsuperscript{7+} ions is relatively broad (FWHM of 40\(^\circ\)-60\(^\circ\)). Similar effects were found for tilt angles as large as 25\(^\circ\).

The latter observation suggests a "guidance" of the Ne\textsuperscript{7+} ion within the capillary \cite{1}, providing evidence that the capillary walls become charged and close collisions with the surface are suppressed. The charge deposition occurs by means of a self-organizing process \cite{1}.

From Fig. 1 it is seen that the transmissions of the ions depend both on the tilt angle and the capillary diameter. Specifically, for 0\(^\circ\) tilt angle the transmissions are about equal for the two capillary diameters, whereas for 15\(^\circ\) tilt angle the transmission through 100 nm capillaries is about an order of magnitude larger than that for 200 nm. This finding strongly supports the picture of ion guiding in the capillary. The higher the aspect ratio of the capillary the higher the capability to bend the ions along the axis of the capillary and transport them to its exit.

Experimental studies of the time evolution \cite{1,2} of the transmission also support the picture of ion guiding, and provide possibility to verify and refine the developed linear \cite{1} and nonlinear \cite{2} self organizing charge deposition models.

![Figure 1. Angular distributions of Ne\textsuperscript{7+} ions transmitted through capillaries in PET. The tilt angle is indicated. Also plotted are data for capillaries in Ag. In (a) and (b) results for capillary diameters of 100 and 200 nm are compared.](image-url)

Acknowledgements

a) Hahn-Meitner Institute Berlin, Glienickerstr. 100, D-14109 Berlin, Germany

b) A significant part of the work was performed during a guest-scientist period in Hahn- Meitner Institute, Berlin.


3.13 Theoretical study of transfer ionization in O\(^{8+}\) + Ar collisions

L. Sarkadi

We continued the theoretical study of the transfer ionization (TI) process in energetic O\(^{8+}\) + Ar collisions. TI is a two-electron process in which the ejection of an electron into the continuum is associated with capture of another electron into one of the bound states of the projectile. Particularly, we are interested in a special kind of TI when the electron is ejected in forward direction with the velocity of the bombarding particle. For such an electron emission the long interaction time with the projectile results in a singularity in the energy spectrum of the electrons, known as ‘electron cusp’. The formation of cusp associated with target ionization is called electron capture to the continuum (ECC). TI proceeding with cusp formation is a special kind of double electron capture: one electron is captured to a bound state, the other electron is captured to a continuum state of the projectile.

TI has been subject of numerous experimental and theoretical investigations, mainly because as a two-electron process it may provide information about the role of electron-electron interaction (correlation) in atomic collisions. The present theoretical work is connected to our previous systematic experimental investigations dealing with cusp-electron emission via TI (for a review see [1]). These studies were carried out with H\(^+\), He\(^+\), He\(^{2+}\), O\(^{7+}\) and O\(^{8+}\) projectile ions in a broad range of the collision velocity (from 4.4 keV amu\(^{-1}\) to 1.5 MeV amu\(^{-1}\)).

We applied the classical trajectory Monte Carlo (CTMC) method to calculate the electron spectra of the cusp peak and the TI/ECC cusp-intensity ratios for 0.3 – 2 MeV amu\(^{-1}\) O\(^{8+}\) + Ar collisions. (We mean ECC ‘pure’ cusp-electron production, i.e., electron emission without bound-state capture.) We carried out the calculations in the independent particle model (IPM) by considering a reduced collision system consisting of the projectile, an active electron and the target ion core. The role of the passive electrons of the target core was taken into account by an effective potential.

Including the contributions of the L and M shell of the Ar target in the calculations, we showed that the maximum observed experimentally [2] in the impact-energy dependence of TI/ECC cusp-intensity ratios is due to the increasing role of the L shell with increasing energy. The obtained results are shown in Fig. 1. In the figure experimental and theoretical data for He\(^{2+}\) ion projectiles are also plotted. CTMC succeeded in the description of the 2TI/ECC ratio, too (2TI: electron emission accompanied by bound-state capture of two electrons).

![Figure 1](image)

Figure 1. Cusp-electron production by TI relative to ECC. Experimental data for O\(^{8+}\) on Ar: full circles, Závodszky et al. [2]; full squares, Breinig et al. [3]. Experimental data for He\(^{2+}\) on Ar: open circles, Víkor et al. [4]. CTMC calculations: solid line, O\(^{8+}\) on Ar (L and M shell, present work); dashed line, He\(^{2+}\) on Ar [1] (M shell only). The \(v_M\) and \(v_L\) Bohr velocities of the M- and L-shell electrons are indicated by vertical lines.

3.14 Interference effects in electron emission from 68 MeV amu$^{-1}$ Kr$^{33+}$ + H$_2$ collisions

L. Sarkadi

We suggest a simple method for the description of the coherent electron emission from the two H atoms of the H$_2$ molecule induced by particle impact. The existence of the interference effect – an analogy of the Young’s two-slit experiment in optics – was demonstrated experimentally by Stolterfoht et al. [1]. Our method is based on a formalism that separates the cross section for the electron emission into an atomic part describing the independent emission from the two H atoms, and a factor giving account of the interference caused by the coherent emission from the two centers:

$$\frac{d^3\sigma_{H_2}}{dq\,d\Omega\,d\epsilon} = \frac{d^3\sigma_{2H}}{dq\,d\Omega\,d\epsilon} \left[ 1 + \frac{\sin(pd)}{pd} \right].$$

(1)

Here $d^3\sigma_{H_2}/dq\,d\Omega\,d\epsilon$ is the triply differential cross section for the electron emission from the H$_2$ target molecule, and $d^3\sigma_{2H}/dq\,d\Omega\,d\epsilon$ is the corresponding cross section for the electron emission from the two H atoms acting as independent particles (denoted by the label 2H). $q$ is the momentum transfer vector defined as the difference between the initial and final momentum of the projectile. The solid angle $d\Omega$ and the energy $d\epsilon$ refer to the ejected electron. The factor in the parentheses describes the interference caused by the coherent emission of the electron from the two H centers. In the interference factor $p$ is the modulus of the vector $p = k - q$, where $k$ is the momentum of the electron. $d$ is the internuclear distance in the H$_2$ molecule. Since in the experiment the vector $q$ was not measured, Eq. (1) has to be integrated over $q$.

The above separability allows the use of a classical ionization theory to determine the atomic part of the cross section. To this we applied the classical trajectory Monte Carlo (CTMC) method. We showed that within CTMC the doubly differential cross section (DDCS) for the molecular electron emission can be evaluated in a very simple way.

Calculations have been carried out for 68 MeV amu$^{-1}$ Kr$^{33+}$ on H$_2$ collisions. A reasonable agreement has been found between the CTMC results and the recent experimental data obtained by Stolterfoht et al. [2], as well as the predictions of the first Born approximation (see Fig. 1).

![Figure 1](https://example.com/figure1.png)

**Figure 1.** Comparison of experimental and theoretical DDCS(H$_2$)/DDCS(2H) ratios as a function of the electron velocity for (a) 30°, (b) 60°, (c) 90° and (d) 150° electron emission angles. The notations: •, experimental data [2] normalized to CDW-EIS [3] atomic cross sections; - - - - , Born approximation [2]; -o-, CTMC (present work).

3.15 Classical description of the fragmentation of positronium in collision with He atoms

L. Sarkadi

Recently Armitage et al. [1] reported on first measurement of absolute break-up cross section for the fragmentation of positronium (Ps) in collision with He atoms in the energy range between 13 and 33 eV. In addition to the measurement of total cross sections, they determined also the longitudinal energy distributions of the emitted positrons. A remarkable feature of the obtained positron spectra is a peak appearing just below 50% of the residual Ps energy \(E_{\text{res}} = E_{\text{Ps}} - 6.8\) eV. The peak was interpreted as an analogy of the electron loss to the continuum (ELC) peak appearing in the energy spectrum of the electrons ejected in the forward direction in ion-atom (atom-atom) collisions. In a previous experiment the related process, electron capture to the continuum (ECC) has been observed by Kővér et al. [2] for positron projectiles.

We applied the classical trajectory Monte Carlo (CTMC) method to the description of the collisional fragmentation of PS. The collision system was simplified to a three-body system consisting of the electron and the positron of Ps, as well as the He atom that was considered as a structureless particle. The interaction of \(e^-\) and \(e^+\) with He was approximated by a static, fully screened Coulomb potential. The calculations were carried out for collision energies 13, 18, 25, and 33 eV. Our theory overestimates the measured total break-up cross sections by a factor of 1.6 – 2.5. At the same time, it correctly reproduces the peak observed in the longitudinal positron spectra (see Fig. 1), supporting a peak formation mechanism similar to the ELC process in atomic collisions.

The dependence of the \(e^-\) and \(e^+\) ejection on the emission energy and angle was also investigated by the CTMC model. A strong \(e^- - e^+\) asymmetry was found for the doubly differential cross sections at low impact energy. This behaviour was explained by the polarization of the Ps atom in the incoming phase of the collision. The asymmetry is expected to diminish at high impact energies.

According to the calculations, a significant \(e^- - e^+\) difference is expected to occur also in the longitudinal energy distributions of the ejected particles. CTMC predicts a peak also in the electron spectrum, but it is less pronounced and shows a larger shift from the expected peak position \(E_{\text{res}}/2\) than the corresponding peak in the positron spectrum. An experiment is suggested in which the longitudinal energy distribution of the electrons emitted in the fragmentation of Ps would be measured.

Figure 1. Longitudinal energy distributions of the positrons emitted in \(\text{Ps} + \text{He}\) collisions for \(E_{\text{Ps}} = 13, 18, 25, \text{and } 33 \text{ eV}\). The experimental data (full circles, Armitage et al. [1]) are normalized to the maxima of the theoretical curves calculated by the present CTMC model. The vertical dotted line shows the expected peak position, \(E_{\text{res}}/2\).


3.16 Transition matrix elements for atomic excitations induced by screened Coulomb potentials

A. Orbán and B. Sulik

In ion-atom collisions the electrons carried by the projectile may influence the target electronic transitions. The electric field created by these electrons screens the Coulomb field of the projectile nucleus. The transition matrix elements, which take into account the screening effect of the projectile are important quantities in the description of such collisions. In the literature, there exist codes, which were built up for calculating matrix elements for the pure Coulomb potential in bound-bound and bound-continuum transitions using hydrogenic wave functions for the atomic states description [1], [2]. Recently, we have published a FORTRAN code [3] which calculates transition matrix elements between atomic bound states with high accuracy as a function of the internuclear distance. Compared with the former codes mentioned above, the present program takes into account the screening effect of the projectile electrons. Moreover arbitrary wave functions, given by the user, can be used for the target atomic states description. We applied the screening model already published in Ref. [4]. For an accurate numerical evaluation of the radial integrals, two main problems appeared. One of them is connected to the fact that in the expression of the screening matrix elements the derivatives of different orders of the modified Bessel functions \( I_{n+1/2}(x) \) and \( K_{n+1/2}(x) \) appear. We developed a relative simple procedure for the calculation of these derivatives, by expressing them with the help of lower order Bessel functions. Consequently, the accuracy of the screening matrix elements depends on the accurate calculation of the modified Bessel functions. We have built up two subroutines for the calculation of these Bessel functions with a relative accuracy better than \( 10^{-10} \) in a wide range of order and argument. The other problem is that the target wave functions are given by the user on arbitrary grid leading to numerical inaccuracies. The radial integral is evaluated in three phases. The integral between 0 and the first non-zero coordinate where the wave function is given by the user is approximated analytically. The remaining two parts of the integral is evaluated numerically, using the equidistant method of Simpson from the first non-zero coordinate to the internuclear distance, and from the internuclear distance to infinity. Detailed tests have been performed at different levels, for different collision systems using hydrogenic wave functions (in tabulated form). For reference, the same calculations have been done by Mathematica [5] using the same wave functions in analytical form. For illustrating the accuracy of the code, we present the results for the dipol transitions \( 1s \rightarrow 2p \) of \( F^{8+} \) ion in collision with He atom in Table 1. The table contains the \( G \) function (the radial part of the integral) for a few internuclear distances, \( R \). The first, second and third rows of the table contain the \( G(R) \) function in the different integration regions while the forth row is the full \( G(R) \) function. In the last column 'valuable digits' indicates the accuracy of the present calculation with respect to Mathematica.

We have also applied the code for the investigation of single excited states of the lithium like oxygen ion [6].

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Table 1. The $G(R)$ function for the $1s \rightarrow 2p$ transition of the $F^{8+}$ ion induced by He projectile.
3.17 Angular distribution of highly charged ions transmitted through metallic microcapillaries

K. Tökési, L. Wirtz\textsuperscript{a}), C. Lemell\textsuperscript{a}), and J. Burgdörfer\textsuperscript{a})

During the last decades studies of interactions between highly charged ions (HCI) and solid surfaces are in center of interest, which is partly stimulated by potential future technical application such as nanofabrication. So far the following picture of the HCI-surface interaction is emerged: When a highly charged ion approaches a solid surface, one or more electrons are resonantly captured at a characteristic distance \(d_c\) into Rydberg states of the projectile. As a result, a multiply excited Rydberg atom with inner shell vacancies, a so-called hollow atom of the first generation (HA1), is created. It is, however, usually extremely short-lived because of the image acceleration of the ion towards the surface. When the ion reaches the surface the memory of HA1 is lost and the hollow atom of the second generation (HA2) is formed. Recently, an alternative technique has been introduced to study HA1s by interaction of highly charged ions with internal surfaces of microcapillaries.

![Figure 1](image)

**Figure 1.** Angular distributions for Xe\textsuperscript{5+} ions for various strength of image acceleration between the ion and the Ni capillary surface at 5 \(\times\) 10\textsuperscript{7} a.u. distance from the capillary exit.

In this work, angular distributions of HA1s creating in microcapillary transmission as function of the interaction strength between the HCI and solid surface are studied. The interaction strength is varied from the case of insulator to the clean metal surface by variation of the surface response function \(\chi = (1 - \varepsilon) / (\varepsilon + 1)\) from small values \(\chi \ll 1\) \((\varepsilon \approx 1)\) to the metallic limit \((\chi \rightarrow 1)\). Here \(\varepsilon\) is the bulk dielectric response. The simulation is based on the classical over the barrier model including the neutralization and relaxation cascade. The electronic dynamics is simulated within a Monte-Carlo approach.

We performed theoretical model calculations for the angular distribution of Xe\textsuperscript{5+} ions with an energy of 800 eV/q transmitted through Ni microcapillaries. We have shown that the angular distributions of transmitted ions can be used to identify different phases of hollow ion formation for clean metal surfaces. We have also investigated the case of surfaces which are partly or entirely contaminated by layers of insulating materials by the reduction of image acceleration. We have found that while the final charge state distributions hardly depend on the strength of the image acceleration the angular distributions change dramatically. Decreasing the image acceleration the angular distribution shifts to the lower scattering angles. Completely neglecting the image acceleration, the angular distribution is centered at zero degree.

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3.18 State selective (n,l) capture distributions in low energy antiproton-helium collisions
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Recently the state selective capture cross sections at very low (1-100 eV) projectile energies were presented in antiproton-helium collisions [1]. The role of isotope effect was also investigated when the capture cross sections for $^3$He and $^4$He targets were compared. These measurements give a sensitive test of various theories when the measured cross sections are compared with the experimental data. The main difficulty in the calculations are caused by the two-center Coulomb field (created by the projectile and target) that influences the motion of the particles. The classical trajectory Monte Carlo (CTMC) method has been quite successful in dealing with capture processes in ion-atom collisions [2,3]. One of the advantages of the CTMC method is that many-body interactions are exactly taken into account during the collisions. This approximation is able to utilize various model potentials between the colliding particles in the same footing.

The state selective (n,l) cross sections for antiproton-capture as a function of impact energy are calculated for $^3$He and $^4$He using the CTMC technique. In the present study a three-body CTMC method [4,5] is used. The potentials representing the interactions between the components of the collision system, the case of Coulomb effective potential (Model 1) and the Garvey-type model potential [5] (Model 2) are considered.

We found the resulting (n,l) distributions of captured antiproton in good agreement with the recent measurements [1] for Model 2. For Model 1, the target potential is described by a point-like Coulomb potential. For this potential the maximum in the n distribution of the captured antiproton is shifted to the higher n values compared to Model 2. This is a strong indication of the importance of screening effect at low energy collisions.

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3.19 Photoionization cross sections of Ne(1s)

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The photoionization cross sections in the energy range between 870 and 1200 eV photon energies of Ne(1s) state are calculated by the independent particle approximation (IPA) \([1,3]\) and by the time dependent density functional theory (TDDFT) \([4,5]\) within the framework of linear density response theory. For the photoionization above the 1s ionization threshold, the dipole transition is dominant. As a test we include the multi-pole contributions in the calculations. We found that the contribution of multi-poles to the total cross sections is less than 0.1 %. Fig. 1 shows the total photoionization cross sections as a function of the photon energy.

\[ \frac{d\sigma}{d\Omega} = \frac{\sigma_T}{4\pi} \left( \sum_l B_1(l) P_l(\cos \theta) + B_2(l) P_l^2(\cos \theta) \cos(2\phi) \right) + \frac{1}{2} P_2^2(\cos \theta) \cos(2\phi) \].

The angular distribution coefficients can be calculated for given effective potentials based on either IPA or TDDFT. Keeping only the dipole transition, Eq. 1 can be simplified for linear polarized photons as

\[ \frac{d\sigma}{d\Omega} = \frac{\sigma_T}{4\pi} \left( 1 - P_2(\cos \theta) \right) + \frac{1}{2} P_2^2(\cos \theta) \cos(2\phi) \],

and for circular polarized photons as

\[ \frac{d\sigma}{d\Omega} = \frac{\sigma_T}{4\pi} \left( 1 - P_2(\cos \theta) \right) \]

respectively. We note that the polarization is chosen on the \(x-y\) plane and the photon is propagated along the \(z\)-direction.

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3.20 The role of projectile double scattering in positron-atom collisions

K. Tőkési

The process of electron capture to the continuum (ECC) can be explained as a result of the special case of ionization, where the ionized target electron is strongly influenced by the outgoing projectile. The ECC peak appears at the energy where the electron velocity is almost the same as the projectile velocity. The ECC is well understood when the projectile is heavy particle. It was shown that the most important mechanism for ECC is the Coulomb focusing of ejected target electron in the direction of the projectile and the peak occur for positron impact as well in the triple-differential cross sections [1]. Since the mass of the positron and the electron is the same, the projectile energy is shared equally between the positron and electron after the ECC. Therefore the nominal value of the ECC peak in the electron/positron spectrum is \( (E - E_b)/2 \). Contrarily, the experimentally obtained positions of the ECC peak always appear at significantly lower/higher energies. To solve this puzzle model calculations within the frame work of classical trajectory Monte Carlo (CTMC) method are performed.


Fig. 2 shows the energy distribution of scattered positrons at 50 eV impact energy when the scattering on the target nucleus is neglected. The ECC peak position is at E=18.2 eV, which is the nominal value at this impact energy. In conclusion we can say that the role of double scattering manifests itself in the energy shift of ECC peak [2].

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3.21 Model calculations for positron-helium scattering

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The comparison between the results of theoretical and experimental investigations of positron–atom scattering provide valuable tests of both the quality of the applied models and wave functions used in the calculations as well as the accuracy of the measured data. Due to the complex nature of the many-body, multichannel collision processes, very detailed theoretical studies of positron scattering by atoms have been made only for H and He (see the recently developed close-coupling calculations of Campbell et al. \cite{1}). On the experimental side, the e\textsuperscript{+}-H system can be studied with great difficulties. In contrast, accurate experimental data have been obtained for He \cite{2,3}. In the case of the e\textsuperscript{+}-He scattering, there are four particles and consequently six inter-particle coordinates. The wave functions of the target are not known exactly. These factors complicate the calculation procedures in comparison with those for e\textsuperscript{+}-H scattering. In order to decrease the complexity of the computational methods, reasonably accurate equivalent one-electron and complex optical model potentials based on optical theory have been proposed for a variety of scattering processes \cite{4,5}.

In the present work we consider the elastic and inelastic scattering of positron from He at energies above the 2\textsuperscript{1}S first excitation threshold at 20.61 eV, i.e. above the Ore gap energy region using a complex optical potential model (COPM) and a classical trajectory Monte Carlo (CTMC) method based on the Garvey-type model potential \cite{6}. It is well known that the optical potential, which replaces the many-channel problem and hence can be used to study the elastic and inelastic scattering mechanism between composite systems, is defined by the Feshbach projection of the Schrödinger equation on a subset from a complete Hilbert–space basis set. The optical potential \(V_{\text{opt}}\) consists of three terms

\[
V_{\text{opt}}(r, E) = V_{\text{stat}}(r) + V_{\text{pol}}(r, E) + iV_{\text{abs}}(r, E),
\]

where \(V_{\text{stat}}\) is the mean static field potential term (MSF) which represents the interaction of the positron projectile with the unperturbed He atom, \(V_{\text{pol}}\) and \(V_{\text{abs}}\) are respectively the polarisation and absorption model potential which can be expressed as a function of the projectile energy \(E\). In Eq. (1) \(r\) is the position vector of the positron with respect to the nucleus. \(V_{\text{pol}}\) has been expanded up to quadrupole order and the precision calculations of Bhatia and Drachman \cite{7} were used for the polarisability coefficients. For the \(V_{\text{abs}}\) potential term we have adopted the expression obtained by Gianturco and Melissa \cite{5}. In our investigations, the MSF potential was derived using three type of wave functions: Hylleraas (H), Hartree–Fock (HF) and one that was constructed from the configuration interaction approximation (CI). The objective is an approximate representation of the ground state of He in order to find out which model is capable of giving accurate data for the elastic scattering cross sections. Since, the non-Hermitian optical potential in Eq. (1) has complex radially symmetric form and short ranged, the partial wave decomposition of the total scattering wave function still makes sense. So, the elastic scattering is described by the regular solution of the

\[
\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_{\text{opt}}(r, E) + k^2 \right] F_l(k, r) = 0, \quad (2)
\]

radial Schrödinger equation, but the \(l\)-th radial wave function \(F_l(k, r)\) is complex. For neutral target systems this regular solution vanishes at the origin and has the following asymptotic behaviour

\[
F_l(k, r \to 0) \to 0, \quad F_l(k, r \to \infty) \to -\sin \left( kr - \frac{lr}{2} + \delta_l(k) \right), \quad (3)
\]
Separating the \( l \)-th partial complex phase shift \( \delta_l(k) \) into its real and imaginary terms, one can write
\[
\delta_l(k) = \lambda_l(k) + i\mu_l(k).
\] (4)

The imaginary component of the phase shift corresponds to absorption, i.e. the loss of particle flux from the incident channel. The total elastic cross section is given according to (for example, Bransden [8])
\[
\sigma_{\text{elas}} = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \left[ \text{ch}\{\mu_l(k)\} - \cos\{2\lambda_l(k)\} \right] \exp\{-2\mu_l(k)\}.
\] (5)

For the numerical solution of the differential equation (2) the modified version of the computer program [9] was used.

**Figure 1.** Elastic integral cross sections for \( e^+ - \text{He} \) scattering.

Figure 1 shows a comparison of calculated elastic cross sections as a function of the positron energy with the previous results obtained by Campbell et al. [1] and Hewitt et al. [10]. We found that the computed cross section is sensitive to the wave function chosen for the approximate description of the ground state of He atom. The obtained values of the COPM-H and COPM-HF cross sections are in a reasonable agreement with the results of the previous quantum mechanical calculations, while the CTMC data overestimates these by a factor of 5. Improvement of the CTMC calculations is planned in the future. The relatively better agreement between the COPM-CI and the multi-state close-coupling data shows that COPM-CI model gives a good account of the elastic scattering process.

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