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Ηλεκτρονική σύλληψη στο συνεχές σε ταχείες κρούσεις πρωτονίων με αέριους στόχους

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Electron capture to the continuum in fast collisions of protons with gas targets

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Ioannina, 2019
To my grandfathers,

Stereos Tampakakis
and
Panagiotis Nanos
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Περίληψη

Στην παρούσα εργασία μελετήθηκε ο ιονισμός αέριων στόχων Ηλίου, Νέου και Αργού από ταχείες δέσμες πρωτονίων ενέργειας 1.5, 3.0 και 4.5 MeV, μέσω της ηλεκτρονικής σύληψης στο συνεχές (μελέτη cusp χορυσμών). Τα πειράματα πραγματοποιήθηκαν στον επιταχυντή 5.5MV tandem Van de Graaff του Ινστιτούτου Πυρηνικής και Σωματιδιακής Φυσικής (ΙΠΣΦ) του ΕΚΕΦΕ "Δημόκριτος" στην Αθήνα. Παράλληλα, πραγματοποιήθηκαν θεωρητικοί υπολογισμοί βασισμένοι στην προσέγγιση διαταραγμένων κυμάτων (CDW-EIS). Κατά αυτόν τον τρόπο έγινε σύγκριση των θεωρητικών υπολογισμών με τα πειραματικά αποτελέσματα. Επίσης, μελετήθηκε η ασυμμετρία των cusp χορυσμών, καθώς και η εξάρτησή τους από τον ατομικό αριθμό του αέριου στόχου \( Z_t \) και την ταχύτητα της δέσμης πρωτονίων \( V_p \). Όπως διαπιστώθηκε, οι θεωρητικοί υπολογισμοί προβλέπουν με καλή ακρίβεια τα πειραματικά αποτελέσματα.

Abstract

The subject of this work is the study of the electron capture to the continuum (ECC) process. We investigated experimentally the corresponding cusp peak in collisions of 1.5, 3.0 and 4.5 MeV protons on He, Ne and Ar gas targets. The experiments were conducted at the 5.5MV tandem Van de Graaff accelerator, located at the National Center for Scientific Research (NCSR) "Demokritos" in Athens. Along with the experimental work, we performed theoretical calculations based on the distorted wave-eikonal initial state approximation. In this way we compared these theoretical calculations with our experimental results. In addition, we studied the asymmetry of the cusp peak and its dependence on the target atomic number \( Z_t \) and the projectile velocity \( V_p \). Overall, our theoretical calculations predict quite well the experimental results.
Chapter 1
Introduction

The process of collisional ionization has been under thorough investigation for several decades, since it plays a vital role not only in our effort to gain detailed knowledge regarding the fundamental structure of matter and the collision dynamics at the smallest scales, but also to provide insight in various scientific fields such as plasma physics [1], thermonuclear fusion research [2], astrophysics [3] and radiotherapy with light ions (hadron therapy) [4]. Hence, understanding basic atomic ionization mechanisms is of increased importance.

Over time, studying the cross sections for ionization of the target atom by the passing projectile ion has been a continuous challenge for both experiment and advanced theories. The main difficulty is attributed to the reaction channels. Electrons ionized from the target atom are not only found in the target's continuum, which is the dominant channel for swift collisions and weak perturbations, but also in bound, or even in low energy continuum states of the projectile for stronger perturbations.

The three main mechanisms that are responsible for the ionization of the target atom from a bare ion give rise to three peaks: (a) the soft electron peak, (b) the cusp electron peak, and (c) the binary encounter electron peak. The soft electron peak arises from glancing collisions, characterized by low energies and momentum transfers. In these collisions the active electron is more influenced by the target atom than the projectile. The qualitative description of the soft electron peak has been developed since the early times of quantum mechanics, and the corresponding dynamics of ionization processes has been perceived. In contrast, to the soft collisions, in the binary collisions the active electron is not interacting with the target atom but rather scatters off the projectile in a head-on collision. In fact, the target only provides the initial velocity distribution of the electron. The resulting ionization process is referred to as binary encounter collision and the corresponding peak as binary encounter.

A third peak, the cusp electron peak, is observed when the emitted electron velocity matches the velocity of the projectile, i.e. when $V_p \approx v_e$. This peak originates from electrons trapped into low-lying projectile continuum states. Depending on the collision system, the cusp electrons may originate from two competing mechanisms. In the first, the active electron is ionized from the target atom and captured into low-energy continuum states of the projectile. This ionization mechanism may proceed with or without the emission of a photon. The first process is known as electron capture to the continuum (ECC), while the second is known as radiative electron capture to the continuum (RECC) [5]. The second mechanism refers only
to non bare projectile where the emitted electron originates from the dressed ion and is ionized into the projectile's continuum during the collision with a target atom. This process is known as electron loss to the continuum (ELC). It is pointed out that the cusp peak is dominated by the ECC and ELC processes in low energy collisions. In addition, electrons originating from ELC can be unambiguously identified only by application of a coincidence condition between the observed electron and the up-charged projectile.

In this work, interest is focused on the ECC process. Early ECC studies triggered research interest due to the orders of magnitude disagreement between the experimental differential cross section data and first order Born approximation calculations. We now know that this divergence arise from the fact that ECC is a two-center process and requires a higher order perturbation theory, as for example the scattering center picture which has been proven to be a powerful concept for the description of the various ionization mechanisms [6-9].

It was 50 years ago since indications of two-center effects were observed [10]. The pioneering work on the ECC peak is attributed to the experimental work of Crooks and Rudd [11], and the theoretical interpretation of Salin [12] and Macek et al. [13, 14]. Since then, numerous experimental data and theoretical treatments have significantly contributed to the understanding of the underlying physics of the cusp electrons. Special reference should be given to Shakeshaft and Spruch for their pioneering theoretical efforts [15-17].

Experiments at tandem Van de Graaff accelerators (TANDEM) with low Z projectile ions and collision energies of few MeV/u allowed for the observation of the contributions of ECC as well as ELC [18-21] processes to the cusp peak. More refined approaches were also taken in studies of ECC as a function of: (a) the electron solid angle acceptance [22], (b) the impact parameter [23], and (c) the target recoil momentum [24]. With the advent of heavy-ion accelerators it became possible to further investigate the collision dynamics of these processes [25-28], testing the limits of the existing theories, and even motivating theorists in developing new ideas for fully relativistic treatments.

Despite the progress in all these years, there are still detailed aspects that require further investigation, even in the nonrelativistic regime. Currently, the most widely used treatment for the ECC peak is the continuum distorted wave-eikonal initial state approximation (CDW-EIS) [29]. It is an improved standard continuum distorted wave approximation (CDW) [30] that better describes the ECC process and which has also been extended to ionization studies [31]. Nowadays, new efforts are in progress to further improve distorted wave theories [32-34].

In the present thesis, experimental data for ECC cusp electrons obtained in collisions of protons with gas targets are presented. The experiments were conducted at the Athens 5.5MV tandem Van de Graaff accelerator at the National Center for Scientific Research "Demokritos" under the Atomic physics with accelerators: projectile electron spectroscopy (APAPES) [35] initiative. In addition, we performed standard CDW-EIS calculations to compare with our experimental findings.
Chapter 2

Theory

2.1 Overview of ionization mechanisms

In this section we present the main ionization mechanisms during collisions of fast (MeV/u) ions with gas targets. In Fig. 2.1 an example of a typical electron spectrum is shown. This spectrum corresponds to the cross section of electron emission at zero degrees with respect to the ion beam, calculated for the collision system of 1.5 MeV $F^{9+} + \text{He}$. The calculations were performed within the Ion-Atom/Argon Program that employs the CDW-EIS approximation. Both the CDW-EIS and the program will be presented in later parts of this thesis.

Figure 2.1: Example of electron spectrum demonstrating the different mechanisms for electron production. The data refer to electron emission at 0° in collisions of 1.5 MeV $F^{9+} + \text{He}$ and were calculated by means of the CDW-EIS approximation with the Ion-Atom/Argon Program.

At the low energy region of the spectrum (lower than 400 eV) the electrons are produced by excitation from a bound target atomic state into a low energy
continuum atomic state of the target atom. This peak area is called the soft electron peak (SC) and the corresponding process soft collisions. At the high energy region of the spectrum (higher than 1100 eV) there is the binary encounter peak (BE). This peak is formed by the binary (head-on) collisions between the target outer electrons and the projectile. The third sharp peak, centered around the energy of 850 eV, corresponding to electron velocities similar to the projectile velocity \( v_e \approx V_p \), is formed due to the capture of target electrons to the low energy continuum of the projectile, known as electron capture to the continuum (ECC).

2.2 Consideration of the two–center electron emission

Over time, it has been realized that the consideration of the electron production in terms of Coulombic centers, which are associated with the heavy nuclei of the collision partners, is a powerful approach. So, instead of working with complex dynamics for the study of a many-body system we can consider the electronic interaction of the heavy centers. The advantage of this lies in the fact that the motion of the heavy centers are independent from the light electrons.

In the Coulombic centers consideration, the formation of a center involves a strong interaction of a nucleus with an active electron. The number of the centers is defined in terms of the accounted interactions of the collision partners with the active electron in the final state. Thus, if the final state includes two interactions, one of the active electron with the projectile nucleus and a second one of the same electron with the target nucleus, then we have a case of a two-center electron emission. This situation is depicted in Fig. 2.2, where the effect of two-center scattering of the emitted electron by both the projectile and the target nuclei is shown.

![Figure 2.2: Schematic illustration of the two-center electron emission process.](image)

The ECC process, which is the main subject of the present work, is a typical example of a two-center effect. From the classical point of view this is easily visualized under the double scattering mechanism postulated by Thomas [36]. Consider a projectile travelling with a speed \( V_p \) towards a target atom. It is found (see Eq. (2.1)) that in a binary collision the target scattered electron has the same velocity with the projectile in case it is scattered at 60° with respect to the projectile trajectory. Then, in a second step, if the electron is elastically backscattered in the field of the target nucleus, it may travel in a trajectory closely parallel to the projectile, thus increasing the probability for capture to low energy continuum states of the projectile. The situation is schematically depicted in Fig. 2.3.
\[ v_e \simeq 2V_p \cos \theta_e \Rightarrow v_e \simeq V_p, \text{ for } \theta_e = 60^\circ. \] 

(2.1)

Figure 2.3: Schematic illustration of the ECC process under the Thomas’s classical double scattering picture.

As it is clear from the previous discussion, the two-center effects are strongly affected by the angular distribution. Thus, the appropriate way to investigate ECC is by means of the double differential cross section (DDCS).

### 2.3 Distorted wave models

The first rigorous theoretical description of the two-center phenomena comes from Salin [12, 37]. In his work, he used an earlier theory [38], initially formulated to study ionization in electron atom collisions, extending it as to include proton impact collisions, predicting the formation of the cusp peak. Until then, the first order Born approximation, that corresponds to single center collision, did not reproduce the cusp peak for the ionization reaction, as shown in Fig. 2.4 for a typical ECC spectrum.

The cusp feature was reproduced only when the initial and the final wavefunctions were treated as distorted from the projectile Coulombic potential. Cheshire [30] introduced such a theory, the CDW approximation, and it was also extended to ionization reaction [31]. The advantage of this approximation lies in the fact that the active electron can be described exactly when the aggregates of the collision system are nearly separated. This asymptotic form behavior of the initial and final collision wavefunctions are given by Eqs. (2.2) and (2.3), respectively:

\[
\lim_{R \cdot v \rightarrow -\infty} \Psi^+ \rightarrow \Phi^B_i \exp \left[ -i \frac{Z_p}{v} \ln (vs + v \cdot s) \right], \quad (2.2)
\]

\[
\lim_{R \cdot v, x, s \rightarrow +\infty} \Psi^- \rightarrow \Phi^{PW}_f \exp \left[ i \frac{Z_i}{k} \ln (kx + k \cdot x) + i \frac{Z_p}{p} \ln (ps + p \cdot s) \right]. \quad (2.3)
\]

The \( \Phi^B_i \) and \( \Phi^{PW}_f \) are the initial and final wavefunctions, respectively, in the free-electron approximation. In this approximation the projectile, the target nucleus and the active electron are treated as free in the exit channel, with the electron
be described by a plane wave. This is a special case of the first order Born approximation. The initial wavefunction is written as:

\[ \Phi_i^B = (2\pi)^{-3} \exp(iK_i \cdot R_i) \phi_i(x), \]  

(2.4)

where the term \( \phi_i(x) \) corresponds to the initial electron wavefunction which describes the electron bound to the target nucleus. The final wavefunction is the:

\[ \Phi_f^{PW} = (2\pi)^{-3} \exp(iK_f \cdot R_i + ik \cdot x). \]  

(2.5)

In the above equations, \( \Psi_i^+ \) and \( \Psi_f^- \) are the CDW incoming and outgoing wavefunctions, respectively, \( Z_p \) is the projectile’s atomic number, \( Z_t \) is the target’s atomic number, and \( p = k - v \) is the final electron momentum vector measured in the projectile rest frame. \( k \) and \( v \) are the momentum vectors of the ejected electron and the impact particle, respectively, with respect to the center of mass of the target. With \( K_i \) and \( K_f \) are denoted the initial momentum vector of the incident reduced particle of mass \( \mu_1 = M_p(M_T + M_e)/(M_p + M_T + M_e) \) and the final momentum vector of the scattered reduced particle of mass \( \mu_2 = M_T(M_p + M_e)/(M_p + M_T + M_e) \). With \( M_T \), \( M_p \) and \( M_e \) are denoted the masses of the target nucleus, the projectile and the electron, respectively. Also, \( x \) is the position vector of the electron and \( s \) is the position vector of the projectile. Both are measured with respect to the target nucleus. Finally, \( R_i \) is the position vector of the projectile with respect to the center of mass of the target atom.

It is worth mentioning that the quantity \( K = K_i - K_f \) expresses the momentum transfer in the center of mass of the system. From the momentum conservation law, we can determine the momentum of the electron in its initial state as \( k_i \approx k - K \). The electron receives a momentum \( K \) due to the collision with the projectile. Thus, the electron is ejected with a final momentum of \( k \approx k_i + K \).
The initial and final distorted wavefunctions, which satisfy the boundary conditions (2.2) and (2.3), were proposed by Belkic [31] and are given in Eqs. (2.6) and (2.7). In these wavefunctions the electron in the entrance channel is considered to move with \(-v\) velocity with respect to the projectile frame in a continuum state of the combined fields of the target nucleus and the projectile. Thus, the final electron continuum state is approximated by a wavefunction that suffers the influence from both the target nucleus and the projectile.

\[
\chi_{i}^{CDW^+} = \Phi_i B N^* \left( \frac{Z_p}{v} \right) {}_1F_1 \left( i \frac{Z_p}{v} ; 1 ; i(vs + \mathbf{v} \cdot \mathbf{s}) \right), \quad (2.6)
\]

\[
\chi_{i}^{CDW^-} = \Phi_i B N \left( \frac{Z_p}{p} \right) {}_1F_1 \left( -i \frac{Z_p}{p} ; 1 ; i(ps + \mathbf{p} \cdot \mathbf{s}) \right). \quad (2.7)
\]

The terms \(N^*(Z_p/v)\) and \(N(Z_p/p)\) are normalization factors, given in Eqs. 2.8 and Eqs. 2.9, which have been chosen to satisfy the boundary conditions, and the \( {}_1F_1(-iZ_p/p; 1; i(ps + \mathbf{p} \cdot \mathbf{s})) \) is the confluent hypergeometric function whose power series expansion is given in Eq. 2.10.

\[
N^*(Z_p/v) = \exp \left( \frac{Z_p \pi}{v} \right) \Gamma \left( 1 - i \frac{Z_p}{v} \right), \quad (2.8)
\]

\[
N(Z_p/p) = \exp \left( \frac{Z_p \pi}{p} \right) \Gamma \left( 1 + i \frac{Z_p}{p} \right), \quad (2.9)
\]

\[
{}_1F_1 \left( -i \frac{Z_p}{p} ; 1 ; i(ps + \mathbf{p} \cdot \mathbf{s}) \right) = \sum_{n=0}^{\infty} \frac{(-iZ_p/p)^n}{n!(1)n^2} [i(ps + \mathbf{p} \cdot \mathbf{s})]^n, |i(ps + \mathbf{p} \cdot \mathbf{s})| < \infty, \quad (2.10)
\]

where \(\sum_{n=0}^{\infty}(a)_n = 1 + a + a(a + 1) + \ldots\).

It is pointed out that the product of the normalization factor with the confluent hypergeometric function is known as Coulomb wavefunction. The Coulomb wavefunctions are defined as particular solutions of the Schrödinger equation in a \(1/r\) potential, and they have been introduced to describe the scattering of charged particles due to the Coulomb repulsion [40].

Despite the fact that the CDW approximation was successful at high collision energies (MeV/u), the approximation failed at lower collision energies. Crothers and McCann proposed that this failure is attributed to the not proper normalization of the CDW initial ansatz. Then, they proposed the replacement of the distorted Coulomb factor in the initial wavefunction with its eikonal approximation [29, 41]. In this improved approximation, only the initial wavefunction is modified accordingly. Thus the CDW-EIS wavefunctions are written as:

\[
\chi_{i}^{EIS^+} = \Phi_i B N^* \left( \frac{Z_p}{v} \right) \exp \left[ -i \frac{Z_p ln(vs + \mathbf{v} \cdot \mathbf{s})}{v} \right], \quad (2.11)
\]

\[
\chi_{i}^{EIS^-} = \Phi_i B N \left( \frac{Z_p}{p} \right) {}_1F_1 \left( -i \frac{Z_p}{p} ; 1 ; i(ps + \mathbf{p} \cdot \mathbf{s}) \right). \quad (2.12)
\]

A brief introductory presentation of the distorted wave models, including the CDW-EIS, can be found in Ref. [42].
The experiments were conducted at the 5.5MV tandem Van de Graaff accelerator, located at the National Center for Scientific Research (NCSR) "Demokritos" in Athens. A schematic illustration of the accelerator is given in Appendix A. A beamline dedicated to atomic collision physics research is located at 45° downstream of the switching magnet (beamline L45) inside the Red target room. In Figs. 3.1 and 3.2 the top view of the TANDEM laboratory and the experimental beamline L45 are shown, respectively.

Here we shall briefly describe our zero-degree Auger projectile spectroscopy (ZAPS) setup illustrated in Fig. 3.3. The setup is composed by the target gas cell and the spectrometer chamber. The spectrometer hosts a hemispherical deflector analyzer (HDA) and is equipped with a 4-element focusing/deceleration entry lens.

Figure 3.1: Top view of the TANDEM laboratory.
and a 2-dimensional position sensitive detector (2D-PSD). The 2D-PSD consists of a typical chevron style 40 mm diameter multichannel plates (MCP) and a resistive anode encoder (RAE). When the projectile ion beam passes through the gas cell it collides with the target atoms. The collision process results in electron production either from the target or the projectile. The emitted at zero-degree electrons are focused by the lens at the entry of the HDA, energy analysed inside the HDA and recorded at the 2D-PSD. The projectile traverses the spectrometer in a straight line due to its higher energy, ending in a Faraday cup (FC) where the beam current is measured. So far, the ZAPS setup was used for projectile and target Auger electron measurements. For a recent description and operation of the setup see Refs. [35, 43].

In Fig. 3.4 a typical 2D spectrum is presented corresponding to cusp electrons measured for 1.5 MeV p + Ne collisions. There, the projections of the 2D image along the x and y axes are shown. The x axis projection is related to the energy of the spectrum and is used for the DDCS determination as we shall present in chapter 4. The y axis projection is related to the overall good focusing conditions of the spectrometer.
Figure 3.4: 2D-PSD image of the ECC in a typical collision of 1.5 MeV p + Ne. [Bottom] x axis projection. [Right] y axis projection.
In this chapter we shall describe the raw data analysis procedure in order to obtain the DDCS. The raw data correspond to the number of electron counts as a function of the channel number of the detector. A typical example of raw data is shown in Fig. 4.1.

Figure 4.1: Typical ECC cusp spectra obtained in collisions of 1.5 MeV proton impact with: (Green triangles) He, (Red squares) Ne and (Blue circles) Ar. The corresponding background measurement is shown with open black squares.

4.1 Energy calibration

The first step in analyzing the data is to convert the channel number to electron energy. This is possible via the energy calibration process. For that, we have to detect electrons at known energies, with the restriction that these electrons were detected under the same experimental conditions as the measurement under study. Electrons can be provided either by an electron gun, or by ion-atom collision Auger
spectra corresponding to well known Auger decay lines. An electron gun can provide electrons at variable kinetic energies with a typical accuracy of 0.1%. On the other hand, known Auger lines, even though they are known with higher accuracy than the electron-gun measurements, they are only available in certain energy regions. In addition, for the determination of the projectile Auger lines, it is necessary to know the beam kinetic energy. This information can be obtained by measuring the maximum value of the cusp peak energy in the electron spectrum.

The relation between the electron energy and the corresponding channel on the 2D-PSD x axis projection is usually a smooth quadratic function, i.e.:

\[ T = a + bi + ci^2, \]  

(4.1)

where \( a, b \) and \( c \) are the calibration constants. It can be shown that:

\[ \frac{T}{W} = \frac{A - 1 + F}{F} + \frac{B}{F^i} + \frac{C}{F^{i2}}, \]  

(4.2)

where \( W \) is the tuning energy of the spectrometer, \( F \) is the deceleration factor and \( A, B \) and \( C \) are the universal calibration constants, i.e. the calibration constants that are a function of \( W \) and \( F \). By comparing Eqs. (4.2) and (4.1) the universal calibration constants \( A, B \) and \( C \) are obtained as:

\[ A = \frac{a}{W}F - F + 1, \]  

(4.3)

\[ B = \frac{b}{W}F, \]  

(4.4)

\[ C = \frac{c}{W}F. \]  

(4.5)

In our case, to calibrate the measured Ne-KLL spectrum shown in Fig. 4.3 the universal calibration constants were obtained by using the known Ne-KLL Auger lines from the bibliography [44]. In detail, by matching four Ne-KLL Auger lines (see Table 4.1), we fitted the corresponding data with a smooth quadratic function according to Eq. 4.1 as shown in Fig. 4.2. This resulted in the calibration constants \( a, b \) and \( c \). It should be mentioned that the calibration measurement was performed at a deceleration factor \( F = 4 \) and a tuning energy \( W = 785 \) eV, while the cusp measurements were performed at a deceleration factor \( F = 1 \). Thus, in order to have the energy calibration for the \( F = 1 \) condition, we used the values of the determined calibration constants and Eqs. (4.3), (4.4) and (4.5), to obtain the universal calibration constants (see Table 4.2).

### Table 4.1: Ne-KLL Auger line energies corresponding to the recorded channels. The Ne-KLL spectrum was recorded at tuning energy \( W = 785 \) and deceleration factor of \( F=4 \).

<table>
<thead>
<tr>
<th>Ne-KLL Auger line</th>
<th>Electron energy (eV)</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K ) (-) ( L_1L_1(1S) )</td>
<td>748</td>
<td>–</td>
</tr>
<tr>
<td>( K ) (-) ( L_1L_23(1P) )</td>
<td>772</td>
<td>62</td>
</tr>
<tr>
<td>( K ) (-) ( L_1L_23(3P) )</td>
<td>782</td>
<td>114</td>
</tr>
<tr>
<td>( K ) (-) ( L_23L_23(1S) )</td>
<td>801</td>
<td>197</td>
</tr>
<tr>
<td>( K ) (-) ( L_23L_23(1D) )</td>
<td>804</td>
<td>211</td>
</tr>
</tbody>
</table>
Figure 4.2: Quadratic fit of the electron energy as a function of the channel number.

Table 4.2: Universal energy calibration constants for $F = 1$ and $F = 4$.

<table>
<thead>
<tr>
<th></th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F = 1$</td>
<td>0.969</td>
<td>$2.166 \times 10^{-4}$</td>
<td>$2.17 \times 10^{-7}$</td>
</tr>
<tr>
<td>$F = 4$</td>
<td>0.875</td>
<td>$8.662 \times 10^{-4}$</td>
<td>$8.66 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

4.2 Double differential cross section

The double differential cross section is a quantity describing the differential in energy and solid angle cross section of a certain process in a collision. The derivation of the DDCS from the experimental raw data is described by the following formula [15]:

$$DDCS_i = \frac{d^2 \sigma_i}{d \Omega dE_i} = \frac{N_{e_i}}{N_I \Delta \Omega \Delta E_i T \eta'},$$

(4.6)

where $i$ refers to the $i$-th channel of the detector. The symbols appearing in the above formula are:

$N_{e_i}$: The number of electron counts at a certain channel $i$ recorded during the measurement.

$N_I$: The number of ions collected at the last FC of the beam line during the measurement. The $N_I$ is calculated as:

$$N_I = \frac{Q(nC)}{q \cdot 1.6 \times 10^{-19}},$$

(4.7)

where $q$ is the ion beam charge state and $Q$ is the total collected charge measured in $nC$ and calculated through experimental parameters as:

$$Q(nC) = \frac{Q_{cnt} I_{FS} (nA)}{C_{nts}},$$

(4.8)
Figure 4.3: Spectrum of the Ne-KLL Auger lines recorded at a tuning energy of $W = 785$ eV and a deceleration factor of $F=4$: (Left) Background subtracted raw counts of the Ne-KLL Auger spectrum as a function of the channel number and (Right) the corresponding energy calibrated spectrum.

where $I_{FS}$ is the current integrator scale in use (CI) measured in $nA$, $C_{nts}$ is the number of counts per second to be generated by the CI when operated to its maximum reading at a certain scale and $Q_{cmi}$ is the number of counts set to the data acquisition system as the upper limit of the total counts to be generated by the CI.

$L$: The effective length of the gas cell:

$$L = L' + \frac{D_1 + D_2}{2},$$

(4.9)

where $L'$ is the actual length of the gas cell and $D_1, D_2$ the entry and the exit nominal diameters, respectively. In our case, $L = 5.175 cm$, since $L' = 5 cm$, $D_1 = 1.5 mm$ and $D_1 = 2 mm$.

$n$: The number of molecules per $cm^3$ at room temperature ($T = 300^\circ K$):

$$n(\#/cm^3) \simeq 3.2 \times 10^{13} P(mTorr),$$

(4.10)

where $P$ is the gas pressure measured in mTorr. For the derivation of Eq. (4.10), we assume that the gas target is an ideal gas, and thus obeys the equation of state $PV = nRT$. According to the pressure values we used for the experiments ($\sim 40 mTorr$) this is an acceptable approximation.

$\Delta \Omega$: The solid angle is determined by the entry lens aperture and the distance
between the gas cell and the lens entry aperture as:

\[ \Delta \Omega = \frac{\pi d^2}{4l^2} \]  \hspace{1cm} (4.11)

where \( d \) is the opening of the lens entrance and \( l \) is the distance between the lens entrance and the center of the gas cell. In our case, \( \Delta \Omega = 1.8 \times 10^{-4} \text{sr} \), since \( d = 4 \text{mm} \) and \( l = 289 \text{mm} \).

\( \Delta E_i \) : The energy step of the spectrum per channel:

\[ \Delta E_i = \frac{dT}{dt} = \frac{W}{F} (B + 2Ci) \]  \hspace{1cm} (4.12)

The energy step is a quite sensitive parameter. Its accurate determination leads to the corrected electron yield and the proper matching of the neighboring spectra slices.

\( T \) : The transmission of the spectrograph. The transmission is defined as the ratio of the number of particles detected at the spectrograph exit (2D-PSD area) divided by the number of particles at the entry of the spectrograph (lens entrance). In our case, the transmission is determined by the three 90\% transmission grids, placed at the exit of the analyzer, as \( T = (0.9)^3 = 0.73 \).

\( \eta \) : The overall efficiency. This quantity corresponds primarily to the MCP detection efficiency \((\approx 55\%)\) as well as any other efficiency factors not properly accounted for during the measurement.

### 4.3 Overall efficiency determination

The overall efficiency was determined by using the Ne-KLL Auger lines in collisions of 3.0 MeV \( p + \text{Ne} \). For the spectrum shown in Fig. 4.4 we recorded two overlapping spectral slices at \( W = 760 \text{ eV} \) and \( W = 785 \text{ eV} \). For the determination of the efficiency we integrated the Ne-KLL Auger peaks and we compared the total area with the corresponding value from Ref. [46]. Thus, we obtained an efficiency value of \( \eta = 0.50 \pm 0.05 \). The uncertainty in this case is due to the total absolute uncertainty of the measurements of Woods et al. [46].

### 4.4 Single collision conditions

In our studies it is important that the measurements were recorded under the scheme of single collision conditions. Under these conditions the projectile ion collides only once with a target atom. Thus, we performed a pressure dependence study to test the single collision conditions. We recorded two measurements at different pressures and compared the resulting normalized data as shown in Fig. 4.5. By increasing the target gas pressure by a factor of two, the normalized counts were also increased by a factor of 2, justifying single collision conditions for pressures smaller than 40 mTorr in the case of Ne gas. Similar studies have been performed for all the collision systems to verify the single collision conditions.
Figure 4.4: Integration of the Ne-KLL Auger lines for the determination of the overall efficiency.

Figure 4.5: Experimental ECC cusp peaks obtained in collisions of 3.0 MeV p + Ar at different target pressures for a pressure dependence study.
Chapter 5

Theoretical calculations

5.1 Angular integration

While comparing our experimental results with our theoretical calculations, based on the CDW-EIS approximation, we realized that the calculated results for zero-degree emission do not fully reproduce the corresponding experimental DDCS. After examining the available ECC cusp bibliography we realized that measurements at similar conditions to ours were scarce. Actually, we found only one ECC cusp measurement for the 1.5 MeV p + He system reported by Lee et al. in Ref. [47], and that was only for energy calibration purposes. Thus, we extracted the data from the above reference and compared them to our measurements finding a fairly good agreement as shown in Fig. 5.1.

![Figure 5.1: Zero-degree DDCS comparison between: (Black dots) the experimental data of Lee et al. [47], (Blue open circles) our measurements and (Red line) CDW-EIS calculations for the collision system of 1.5 MeV p + He.](image)

Actually, our spectra are broader than Lee’s. We attribute this behavior to
the larger detection solid angle of our spectrometer setup compared to the tandem parallel plate analyzer (PPA) used by Lee et al. This explanation is supported by the report in Ref. [48].

Thus, we extended the CDW-EIS calculations as to include the angular spread of the detection solid angle of our setup, corresponding to $\Delta \theta = 0.8^\circ$. For this we performed integrations at various angular binnings as presented in Fig. 5.2. We found that the agreement was improved in the energy region around the cusp peak. In general, the net zero-degree calculation exceeds the cusp peak cross section of our data but the integrated calculation results in a lowering of the cusp peak cross section as shown in Fig. 5.2.

Next we shall present the process of integration in our calculations. The DDCS for the ECC cusp peak is strongly depended on the angle of electron emission. Thus, we performed a normalized summation over a number of angles covering our detection solid angle, described by the following equation:

$$\frac{d^2\sigma}{\Delta \Omega dE} = \frac{\sum_i \frac{d^2\sigma}{d\theta_i dE} (\theta_i) \Delta \Omega_i}{\sum_i \Delta \Omega_i}. \quad (5.1)$$

We also know for the solid angle that [49]:

$$\Delta \Omega_i = 2\pi (\cos \theta_i - \cos \theta_{i+1}). \quad (5.2)$$

Combining the Eqs. (5.1) and (5.2) the solid angle integrated DDCS resulted in:

$$\frac{d^2\sigma}{\Delta \Omega dE} = \sum_i \frac{d^2\sigma}{d\Omega_i dE} (\theta_i) \left( \frac{\cos \theta_i - \cos \theta_{i+1}}{1 - \cos \theta_{max}} \right) . \quad (5.3)$$
As can be seen, the integrated DDCS is the sum of individual DDCSs corresponding to all infinitesimal angles, covering the experimental solid angle, multiplied by the corresponding areal statistical factors. We tested the appropriate number of angles in use for the 1.5 MeV $p + \text{He}$ collision system. As it shown in Fig. 5.2, dividing the experimental solid angle in 10 angular steps is a satisfactory condition for both quick and precise calculations.

5.2 $l$-subshell contribution

The Ion-Atom/Argon Program provide us the ability to calculate the contribution of the $l$-subshells in the DDCS. In our case, we calculated all the available $l$-subshells for the collision systems under study separately. Then we obtained the final DDCSs by adding the corresponding $l$-subshells statistically $[2(2l + 1)]$, i.e. we multiplied the resulted $l$-subshell DDCSs by the corresponding maximum number of electrons.

This process was necessary, since the ECC cusp peak strongly depends on the electron velocities of the target, i.e. the Compton profile of the target. The ECC cusp peak is favored for electron velocities close to that of the projectile. Thus, different beam energies correspond to different $l$-subshell contributions. These contributions are shown in Figs. 5.3 and 5.4 for the cases of proton impact on Ne and Ar, respectively, at projectile energies of 1.5, 3.0 and 4.5 MeV. There, the variation of the $l$-subshell contribution is shown.

For the case of Ne when the proton energy is 1.5 MeV the main contribution to the final DDCS comes from the 1s and 2p orbitals. However, as the proton energy increases, the contribution from the 2p orbital becomes significantly weaker. The situation in the case of Ar is more complicated since we have 5 orbitals to compare with. For 1.5 MeV proton energy the larger contribution comes from the 2p orbital while the smaller contribution comes from the 1s orbital. The 2s, 3s and 3p orbitals give roughly the same contribution to the final DDCS. However, as the energy increases, the contribution from the 1s orbital also increases while the contribution of the 3p and the 3s orbitals is reduced. In all the energies, the 2p orbital contributes the most to the final DDCS. From this analysis we conclude than in the case of Ne the main contribution to the DDCS comes from the K-shell, while for the case of Ar the main contribution comes from the L-shell.
Figure 5.3: $l$-subshell contribution to the ECC cusp DDCS in collisions of: (Left) 1.5 MeV p + Ne, (Middle) 3.0 MeV p + Ne and (Right) 4.5 MeV p + Ne. The different line colors indicate different orbitals: (Blue line) 1s, (Red line) 2s and (Green line) 2p.

Figure 5.4: Same as Fig. 5.3 but for Ar gas target. The different line colors indicate different orbitals: (Blue line) 1s, (Red line) 2s, (Green line) 2p, (Purple line) 3s and (Black line) 3p.
Chapter 6

Results and discussion

In this chapter, the experimental results on ECC cusp electrons production along with the CDW-EIS calculations are presented. The collision systems under discussion are the 1.5, 3.0 and 4.5 MeV proton impact on He, Ne and Ar gas targets. The calculations were performed using the Ion-Atom/Argon Program presented in Appendix B. After the presentation of the results we proceed to a detailed discussion about the comparison between the CDW-EIS calculations and the experimental results, the asymmetry, and the $Z_t$ and $V_p$ scaling laws of the ECC cusp peak.

6.1 Experimental results and CDW-EIS calculations

We started by investigating the ECC cusp production of the collision systems 1.5 MeV $p +$ He, Ne and Ar gas targets. This is the lowest available collision energy offered by the TANDEM accelerator and thus corresponds to the highest cross section for the He gas target compared to the other higher energy collisions, presented later on. It is worth mentioning here that the case of He corresponds to a collision including four bodies and for this reason is of increased interest for developing detailed distorted wave theories as for example the four-body distorted wave-eikonal initial approximation (4B-DW-EIS) \cite{32,33}. The experimental results are presented in Fig. 6.1 along with the solid angle integrated CDW-EIS calculations. As it shown, the CDW-EIS calculations are reproducing quite well the experimental ECC cusp peak maximum for the cases of Ar and Ne. Concerning the experimental results for the He case though, we see a higher cusp peak value from that calculated with CDW-EIS.

We also investigated the ECC cusp in collisions of 3.0 MeV $p +$ Ne and Ar gas targets. In this energy we did not observe the ECC cusp peak for the He gas, due to the very low production cross section at this collision energy. However, we performed the corresponding CDW-EIS calculation. The results are presented in Fig. 6.2. As it is shown, theory is in a quite good agreement with the experimental results for the cases of Ar and Ne. Not only the cusp peak maximum values were predicted from the calculations, but also the cusp wings were found in better agreement with the measurements than in the previous case.

Finally, we investigated the ECC cusp in collisions of 4.5 MeV $p +$ Ne and Ar gas targets. The case of He at this beam energy was studied only theoretically. The results are presented in Fig. 6.3. As in the previous case, the CDW-EIS results are in a quite good agreement with experiment.
Figure 6.1: ECC spectrum obtained in collisions of: (Left) 1.5 MeV p + He, (Middle) 1.5 MeV p + Ne and (Right) 1.5 MeV p + Ar. The experimental data are shown with blue dots while the CDW-EIS calculations with red lines.

Figure 6.2: Same as Fig. 6.1 but for 3.0 MeV proton impact.
Figure 6.3: Same as Fig. 6.1 but for 4.5 MeV proton impact.
6.2 Cusp wings

As it is evident from the previous analysis, there are cases where a discrepancy is observed between the CDW-EIS calculations and the experimental data in the cusp wings. In more detail, in these cases the CDW-EIS calculations underestimate the cross section in the cusp wings even though an angular integration was included in the calculations. However, it is reported in the literature that sophisticated distorted wave theories like the four-body distorted wave approximation provide better agreement. Indeed, in Fig. 6.4 we present the 4B-DW-EIS calculation taken from Monti et al. [32], along with the standard three-body CDW-EIS calculation that we performed, and the experimental data of Lee et al. [47], for the collision system 1.5 MeV p + He. As it is shown, the more refined results of the 4B-DW-EIS reproduces the experimental data more than satisfactorily.

Figure 6.4: ECC cusp spectra for the collision system of 1.5 MeV p + He: (Open circles) Experimental DDCS taken from Lee et al. [47], (Green line) 4B-DW-EIS calculation taken from Monti et al. [32], (Red line) CDW-EIS calculation performed with the Ion-Atom/Argon Program.
6.3 Peak asymmetry of the ECC cusp

Since the early years of the cusp peak study it has been found that the ECC cusp peaks are skewed in the low energy wing [22, 50, 51]. The cusp asymmetry observations were first theoretically explained when the second-order Born term was taken into account in the calculated ECC differential cross sections [10]. This asymmetry is related to the final state of electrons, where the two-center field of the projectile and the target nucleus are playing an important role. The explanation can be visualized in the projectile rest frame, where the captured electron is dragged backwards by the target field.

The skewness in the low energy wings was also visible in the ECC cusps presented in this work. In Fig. 6.5 we show the ECC cusp wing asymmetries. In these graphs the x axis is the cusp wing absolute energy, i.e. the energy width of the cusp wings (absolute energy = |E_i - E_{cusp}|). As it is shown, the widths of the low energy wings are wider for all the cases, as we expected based on the nature of the asymmetry, i.e. the attraction that the electron suffers by the receding target ion.

Figure 6.5: Presentation of the asymmetry for all the ECC cusp spectra obtained in the present work. In these graphs the ECC cusp peaks obtained experimentally in collisions of: (Left column) 1.5 MeV p + He, Ne, Ar, (Middle column) 3.0 MeV p + Ne, Ar and (Right column) 4.5 MeV p + Ne, Ar are presented. The low energy cusp wings (E_{low} = |E - E_{cusp}|) are shown with red squares and the high energy cusp wings (E_{high} = E - E_{cusp}) with green circles.

Information about the cusp asymmetry was extracted from the full widths at
half maxima (FWHM) of the DDCS spectra. For the FWHM determination we subtracted a statistical background from the DDCSs and we fitted the resulted peaks with split Lorentzian distributions. Thus, we obtained the ratio $W_L/W_H$, i.e. the asymmetry factor, where the terms $W_L$ and $W_H$ are referring to the FWHM of the low and the high energy wing, respectively. The resulted asymmetry factors are given in Table 6.1 and are also presented in Fig. 6.6. As we see, the asymmetry factors seem to slightly decrease with increasing projectile velocity. This indicates a smaller asymmetry for higher collision energies. This can be interpreted as a smaller effect of the electron pull by the target atom due to higher velocities or equivalently and classically speaking due to higher interaction times.

Table 6.1: Experimental asymmetry factors $W_L/W_H$.  

<table>
<thead>
<tr>
<th>$W_L/W_H$</th>
<th>He</th>
<th>Ne</th>
<th>Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5 MeV</td>
<td>2.3 ± 0.3</td>
<td>2.0 ± 0.2</td>
<td>1.9 ± 0.2</td>
</tr>
<tr>
<td>3.0 MeV</td>
<td>−</td>
<td>1.9 ± 0.2</td>
<td>1.8 ± 0.2</td>
</tr>
<tr>
<td>4.5 MeV</td>
<td>−</td>
<td>1.6 ± 0.1</td>
<td>1.6 ± 0.1</td>
</tr>
</tbody>
</table>

Figure 6.6: Asymmetry factors as a function of the projectile velocity for collisions of: (Red square) 1.5 MeV p + He, (Green circles) 1.5, 3.0, 4.5 MeV p + Ar, Ne and (Blue triangles) 1.5, 3.0, 4.5 MeV p + Ar, Ne.
6.4 Scaling laws

Next, we study the dependence of the ECC cusp peak on the atomic number of the gas target \( Z_t \) and the velocity of the projectile \( V_p \) in search of scaling laws. For the study of the \( V_p \) dependence we calculated the projectile velocity relativistically:

\[
V_p (\text{mm/ns}) = c(\text{mm/ns}) \cdot \sqrt{1 - \frac{1}{\left(1 + \frac{E_p(\text{MeV/u})}{E_e(\text{MeV/u})}\right)^2}}, \tag{6.1}
\]

where \( c \) is the speed of light in \( \text{mm/ns} \), and \( E_p \) and \( E_e \) are the energy of the projectile and the electron, respectively, in \( \text{MeV/u} \).

For this study, we obtained the single differential yields (SDY) of the cusp peaks by integrating the DDCSs over the energy, after subtracting the background. Applying different backgrounds in the analysis (linear and quadratic) we determined for both theoretical and experimental SDYs an uncertainty of 10%. This value contains the systematic uncertainties which are coming from the determination of the DDCS and are less than 1%.

For the \( Z_t \) scaling law case, the compared spectra were recorded over the same energy width. However, for the \( V_p \) scaling law case, we had to compare spectra that have been measured at different collision energies and thus have been recorded at different energy widths. So, the SDYs were obtained after integration of the spectra over a fixed range of 150 eV energy width for all the cases. In this way we were able to systematically compare the SDYs resulted from different proton impact velocities.

6.4.1 ECC dependence on target atomic number \( Z_t \)

We begin by investigating the scaling law of the ECC cusp peaks as a function of the target atomic number \( Z_t \). It is known that the dependence of the ECC cusp on target atomic number is expressed by a scaling law in the form of \( Z_t^\alpha \) \[13, 19, 52\]. In order to determine the \( \alpha \) parameter we obtained the ratios shown in Table 6.2. According to these values we found the \( \alpha \) parameter, both for theory and experiment, as follows:

\[
\alpha = \frac{\log(Y_1/Y_2)}{\log(Z_{t1}/Z_{t2})}. \tag{6.2}
\]

The results are presented in Table 6.3.

Table 6.2: Experimental and theoretical ratios of the ECC cusp SDYs for different gas targets at the same collision energy.

<table>
<thead>
<tr>
<th>Ratio</th>
<th>1.5 MeV</th>
<th></th>
<th>3.0 MeV</th>
<th></th>
<th>4.5 MeV</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( Y(Ar)/Y(Ne) )</td>
<td>2.6</td>
<td>4.0</td>
<td>2.7</td>
<td>3.4</td>
<td>2.3</td>
<td>2.9</td>
</tr>
<tr>
<td>( Y(Ne)/Y(He) )</td>
<td>15.0</td>
<td>25.9</td>
<td>-</td>
<td>108.3</td>
<td>-</td>
<td>241.7</td>
</tr>
<tr>
<td>( Y(Ar)/Y(He) )</td>
<td>39.3</td>
<td>104.4</td>
<td>-</td>
<td>364.9</td>
<td>-</td>
<td>693.5</td>
</tr>
</tbody>
</table>

We see that the experimental ratio \( Y(Ar)/Y(Ne) \) is fairly constant for all the energies. On the other hand, the corresponding CDW-EIS ratios are seen to be reduced...
with increasing energy. The remaining two ratios were determined only for the case of 1.5 MeV proton impact, since we do not have experimental data for the He gas in the other two energies. In this case, the experimental results and the theoretical predictions for the $Y(1.5 \text{MeV})/Y(He)$ and $Y(3.0 \text{MeV})/Y(He)$ ratios deviate significantly. This disagreement is supported from the discrepancy in the DDCS between theory and experiment in the case of He, as it is clearly shown in Fig. 6.1 and does not come as a surprise.

Table 6.3: Determination of the experimental and the theoretical target atomic number scaling law parameter ($\alpha = \log(Y_1/Y_2)/\log(Z_{t1}/Z_{t2})$).

<table>
<thead>
<tr>
<th>Ratio</th>
<th>1.5 MeV</th>
<th>3.0 MeV</th>
<th>4.5 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Ar : Ne$</td>
<td>1.6 ± 0.5</td>
<td>2.4 ± 0.6</td>
<td>1.7 ± 0.6</td>
</tr>
<tr>
<td>$Ne : He$</td>
<td>1.7 ± 0.2</td>
<td>2.0 ± 0.2</td>
<td>—</td>
</tr>
<tr>
<td>$Ar : He$</td>
<td>1.7 ± 0.2</td>
<td>2.1 ± 0.2</td>
<td>—</td>
</tr>
</tbody>
</table>

The results about the $\alpha$ parameter are shown as a function of the corresponding atomic number ratio in Fig. 6.1. We see that experiment and theory are in a fairly good agreement as concerning the $Z_t$ scaling law. The experimental parameter $\alpha$ is determined, as an average of all the experimental values, $\alpha = 1.6 \pm 0.1$. The theoretical value of $\alpha$ seems to vary in the range of $\alpha = 1.8 - 3.4$.

6.4.2 ECC dependence on projectile velocity $V_p$

The cross section of the ECC cusp peak also depends on the projectile velocity $V_p$. As it was shown from the previous analysis, the ECC cusp decreases with increasing velocity, so the corresponding scaling law is in the form of $V_p^{-\beta}$ [19, 52]. The necessary ratios for the determination of the $\beta$ parameter were extracted from the cusp SDYs and are shown in Table 6.4.

Table 6.4: Experimental and theoretical ratios of the ECC cusp SDYs for the same gas atomic target at different collision energies.

<table>
<thead>
<tr>
<th>Ratio</th>
<th></th>
<th>He</th>
<th>Ne</th>
<th>Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y(1.5 \text{MeV})/Y(4.5 \text{MeV})$</td>
<td>Exp.</td>
<td>Theor.</td>
<td>Exp.</td>
<td>Theor.</td>
</tr>
<tr>
<td>$Y(1.5 \text{MeV})/Y(3.0 \text{MeV})$</td>
<td>—</td>
<td>233.8</td>
<td>29.8</td>
<td>27.0</td>
</tr>
<tr>
<td>$Y(3.0 \text{MeV})/Y(4.5 \text{MeV})$</td>
<td>—</td>
<td>28.5</td>
<td>7.9</td>
<td>6.9</td>
</tr>
</tbody>
</table>

As can be seen, in this case we have results only for the Ne and Ar gases. We see that the theoretical ratios are in a quite good agreement with the corresponding experimental ratios. From the ratios shown in Table 6.4, we obtain the $\beta$ parameter both for theory and experiment, as follows:

$$\beta = -\frac{\log(Y_1/Y_2)}{\log(V_{p1}/V_{p2})}. \quad (6.3)$$

The results are presented in Table 6.5 and in Fig. 6.8 as a function of the corresponding projectile velocity ratios.
Table 6.5: Determination of the experimental and the theoretical projectile velocity scaling law parameter ($\beta = -\frac{\log(Y_1/Y_2)}{\log(V_{p1}/V_{p2})}$).

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>He</th>
<th></th>
<th>Ne</th>
<th></th>
<th>Ar</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5 MeV:4.5 MeV</td>
<td>10 ± 1</td>
<td></td>
<td>6 ± 1</td>
<td></td>
<td>6 ± 1</td>
<td></td>
</tr>
<tr>
<td>1.5 MeV:3.0 MeV</td>
<td>10 ± 1</td>
<td></td>
<td>6 ± 1</td>
<td></td>
<td>6 ± 1</td>
<td></td>
</tr>
<tr>
<td>3.0 MeV:4.5 MeV</td>
<td>10 ± 2</td>
<td></td>
<td>7 ± 3</td>
<td></td>
<td>6 ± 2</td>
<td></td>
</tr>
</tbody>
</table>

We see that in this case CDW-EIS predictions agree quite well with the experimental results. Both theory and experiment give a $\beta$ value in the range of $\beta = 6 - 8$, except from the case of He where theory predicts a $\beta$ of 10. Thus, an experimental value of $\beta = 6 \pm 1$ is established.
Figure 6.7: (Squares) Experimental and (Circles) theoretical $\alpha$ parameters as a function to the corresponding atomic number ratios ($Z_{t1}/Z_{t2}$). The results were obtained in collisions of: (Left) $1.5$ MeV $p +$ He, Ne, Ar, (Middle) $3.0$ MeV $p +$ He, Ne, Ar and (Right) $3.0$ MeV $p +$ He, Ne, Ar.

Figure 6.8: (Squares) Experimental and (Circles) theoretical $\beta$ parameters as a function to the corresponding projectile velocity ratios ($V_{p1}/V_{p2}$). The results were obtained in collisions of: (Left) $1.5, 3.0, 4.5$ MeV $p +$ He, (Middle) $1.5, 3.0, 4.5$ MeV $p +$ Ne and (Right) $1.5, 3.0, 4.5$ MeV $p +$ Ar.
6.5 Overall view of the results

Finally, we gather all the information obtained in the present work in Fig. 6.9. There, our results are presented in an illustrative way that helps the reader to visually realize: (i) how well does CDW-EIS calculations predict the experimental ECC cusp peaks, (ii) the dependence of the ECC cusp peak DDCS on the atomic number of the target and the velocity of the projectile velocity, and (iii) the asymmetry of the ECC cusp peaks.

Figure 6.9: Presentation of all the ECC cusp spectra obtained in this work. The ECC cusp peaks were obtained both experimentally (shown with shapes) and theoretically (shown with lines) in collisions of: (Left) 1.5 MeV p + He, Ne, Ar, (Middle) 3.0 MeV p + He, Ne, Ar and (Right) 4.5 MeV p + He, Ne, Ar. The different colors indicate the different gas targets: Blue for Ar, red for Ne and green for He.
Chapter 7

Summary and conclusions

In this final chapter we summarize the results of the study of the electron capture to the continuum process. We investigated experimentally the ECC cusp peak in collisions of 1.5, 3.0 and 4.5 MeV protons on He, Ne and Ar gas targets. The experiments were conducted at the 5.5MV tandem Van de Graaff accelerator, located at the National Center for Scientific Research (NCSR) "Demokritos" in Athens. Along with the experimental work, we performed theoretical calculations based on the distorted wave-eikonal initial state approximation. In these calculations the angular spread of the detection solid angle of our setup has been considered. In addition, the l-subshell contributions of the orbitals of all the targets in use were included in the calculations. An overall good agreement with experiment has been found. Furthermore, we studied the asymmetry of the ECC cusp peak and found that its shape changes smoothly for our collision systems. Then, we determined the dependence of the ECC cusp peak on the target atomic number $Z_t$ and the projectile velocity $V_p$. We determined the scaling laws from our experimental results as $Z_t^{1.6\pm0.1}$ and of $V_p^{-6\pm1}$. From this study it becomes evident that more refined distorted wave approaches have to be considered for the ECC process.
Chapter 8

Future prospects

Despite the insight we gain about the ECC cusp mechanisms, more studies are required in order to better understand the physical processes in play. For that reason, here we present our suggestions.

We first propose the investigation of the ECC cusp wings for the collision systems that we presented in this thesis, i.e. 1.5, 3.0 and 4.5 MeV p + He, Ne and Ar. For this study, we need to take various measurements in different overlapped spectral slices. After this study, we will be able to obtain more information about the shape of the ECC cusps, thus we will be able to extract more refined results about the asymmetry and the scaling laws of the ECC cusp peaks.

We also propose to extend our ECC studies by performing experiments with deuteron beams. This idea stems from the fact that deuterons at collision energies of 1.5 MeV are equivalent to protons at collision energies of 750 keV. This energy is not offered by the tandem accelerator where our experiments were conducted. Among others, it is important that using deuterons of 1.5 MeV will make possible the observation of both ECC and BEE peaks in a common spectrum. We believe that this effort has to be done for the most interesting case of He gas for comparison reasons with the available theories. Finally, we will be able to observe the ECC cusp peak in collisions of 1.5 MeV d + H₂.

Also, we would like to investigate the angular distribution dependence of the ECC cusp peak DDCS by decreasing the solid angle of our ZAPS setup. For this study we need to set up an iris (aperture of variable diameter) in front of the spectrometer’s entry.

Finally, we believe that it will be interesting to investigate ECC cusp peaks in collisions of gas targets with mixed state beams. Such experiments have already taken place with He-like beams at low energy collisions [53-55]. However, an extension of these studies will enable us to further investigate the ECC cusp contribution from the ¹S and the ³S components.
Acknowledgments

The present work would not have been accomplished without the support and the inspiration from various people. Here, it is given me the opportunity to express my sincere thankfulness to all of them.

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Appendix A

Accelerator description

In Figs. A.1 and A.2 are presented a panoramic view and a schematic illustration of the 5.5MV tandem Van de Graaff accelerator, respectively. The numbers shown in Fig. A.2 refer to the different main parts of the accelerator. These parts are presented below in short:

0. Source and pre-acceleration controls (power supplies, misc. electrical units)
1. Sputter source
2. Duoplasmatron source
3. Box lens (powered by common PS)
4. Inflector magnet
5. Einzel lens 1
6. Low energy slits
7. Low energy cup
8. Quartz
9. Low energy steerers (4 pairs)
10. Einzel lens 2
11. Tank
12. In-tank steerer
13. Charge-stripping carbon foil
14. Resistances
15. Hollow metal sphere
16. Corona
17. Belt
18. Belt upcharging power supply
19. Pulleys
20. Screens
21. High energy cup
22. High energy quadrupoles (x2)
23. High energy steerers (4 pairs)
24. High energy slits
25. Analyzing magnet
26. Analyzer slits
27. Analyzer cup
28. Analyzer quadrupole (x2)
29. Switching magnet
Figure A.1: Panoramic view of the 5.5MV tandem Van de Graaff accelerator.

Figure A.2: Schematic illustration of the 5.5MV tandem Van de Graaff accelerator.
Appendix B

Ion-Atom/Argon Program

The Ion-Atom/Argon Program [57] is a free to download FORTRAN 90 program which calculates the total, single and double differential cross sections for the single target ionization of neutral atoms ranging from hydrogen up to argon by the impact of fully stripped ions. The code is applicable for the case of both high and low Z projectile impact in fast ion-atom collisions. The program is equipped with two theoretical models, the CDW and CDW-EIS approximations. The present program extend previously published codes for single ionization of target hydrogen [58], target helium [59] and target atoms ranging from lithium to neon [60].

In this Appendix we are presenting step by step the procedure for a calculation. For this purpose we are using as an example the calculation of the DDCS for 1.5 MeV $F^{9+}$ collision on He at 0 degrees:

We start by opening the ARGON_DRIVER.f90 where we give the input data. The environment of the program is presented in Fig. B.2. Below, we are presenting the inputs in the order in which they are requested from the code. In parenthesis we are giving the corresponding input that we gave for this exemplary calculation.

- The code asks first to choose the gas target. (We chose 1 for He target).
- Then, we have to choose the theoretical approximation which the program will use for the calculation. (We chose 2 for CDW-EIS.)
- After that, we have to choose the type of the cross section that we want to calculate. (We chose 2 for DDCS.)
- Next comes the $l$-subshell to be considered. (We chose 1 for the 1s subshell.)
- Afterwards, we have to give the projectile charge. (We chose 9 for Fluorine. We remind that the program treats the projectile ions as fully stripped so with our choice we have a $F^{9+}$ projectile.)
- Then, the program asks to give the starting value, the upper limit and the increment value for the ejected electron energy in eV (We chose our energy interval to be from $10\text{eV}$ to $5000\text{eV}$ and also we chose the increment value to be $1\text{eV}$ for a precise calculation.)
- The next input is the energy of the projectile in keV/u. (We chose 1500 keV/u.)
• Before the end we have to choose the value for the polar angle of emission for the ejected electron in radians (We chose 0 since we want our calculation to be performed for 0 degrees.)

• Finally, we have to enter a tolerance value, used for the integration. This quantity set a lower bound on tolerances required for numerical routines. (We chose 1E-8 for a high precision in our calculation.)

After giving the necessary inputs, the info_total file is generated in which the information that we gave is stored. Then we run the ARGON.f90 and the calculation procedure starts. A window like that shown in Fig. B.1 appears on the screen until the calculation is over.

![Figure B.1: Pop up window of the ARGON.f90 application during the calculation.](image)

After finishing the calculation, the theoretical data are stored into two files. The first file holds all the information about our calculation, both the inputs and theoretical data, and is called total_output. The second file is called raw_data. In this file are only stored the theoretical values. Both files can be opened by any simple text editor. Part of these files corresponding to our example are presented in Figs. B.3 and B.4.

Our theoretical values taken for the needs of this example are presented in Fig. B.5. Along with our calculation there is a previous CDW-EIS calculation taken from Schultz and Reinhold [61] and experimental data taken from Lee et al. [47]. As it is shown, the calculation matches the previous one giving us the conviction that the calculations we made for the needs of the present work are reliable. We also see that the CDW-EIS approximation is in a quite good agreement with experiment, thus justifying why this model is very successful in the study of ionization in ion atom collisions.
Figure B.2: Exemplary calculation in the ARGON_DRIVER.f90 environment.
Figure B.3: Part of the total_output file corresponding to the example.

Figure B.4: Part of the raw_data file corresponding to the example.
Figure B.5: DDCS of the collision system 1.5 MeV \( F^{9+} + \text{He} \) at 0° emission angle: (Red line) Our theoretical values were calculated with the Ion-Atom/Argon Program using the CDW-EIS approximation. This calculation is compared with (Green line) a previous CDW-EIS calculation of Schultz and Reinhold [61] and (Blue dots) experimental data of Lee et al. [47].
Bibliography


