Atomic ionization by multicharged ions interpreted in terms of poles in the velocity complex space

J E Miraglia

Instituto de Astronomía y Física del Espacio, Consejo Nacional de Investigaciones Científicas y Técnicas, Buenos Aires, Buenos Aires 1430, Argentina

E-mail: miraglia@iafe.uba.ar

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Abstract
We study the single ionization of hydrogen and helium by the impact of a highly charged Coulomb projectile. To interpret the cross section we introduce a diagonal Padé approximant. We find that the use of a Padé \([4, 4]\) describes the continuum distorted wave eikonal initial state theory within its range of validity very well. The nodes of the denominator of the Padé approximant give rise to four poles in the velocity complex plane: two in the upper plane and their conjugates in the lower plane. The dependence of these poles with the projectile charge can be reasonably fitted to give a closed form for the ionization cross section, resulting in a scaling very near to that of Janev and Presnyakov. The experiments available were described very well in its entire velocity range with the use of a Padé \([8, 8]\), with four poles in the upper plane and their conjugates in the lower plane. We conclude that the poles of the Padé approximant seem to have all the information of the total ionization cross section.

Keywords: ionization, atoms, scaling

(Some figures may appear in colour only in the online journal)

1. Introduction

With the advancement of the big accelerators, the subject of ionization of atoms by highly charged ions has developed notably. It was accompanied with the development of several quantum and classical theories, for example, the distorted waves such as the continuum distorted wave eikonal initial state (CDW for short) \([1]\), the classical trajectory Monte-Carlo (CTMC) \([2]\), and close coupling calculations such as the basis-generator method (BGM) \([3]\), among others. For many-electron atoms the situation is certainly very complex due to several mechanisms involved, including several electron transitions. But even with simple targets such as hydrogen and helium, the experiments are limited. Still there is no theory that can predict with certainty the ionization of these simple systems for a large charge of the projectile \(Z\) and for a given impact velocity \(v\). In fact, the only theoretical method that has consistently accompanied most of the experiments has been the CTMC; its simplicity, ubiquity and applicability makes this classical method a favorite tool to deal with large \(Z\). The quantum CDW theory is a very useful and reliable tool, but its validity is reduced to the intermediate high-energy region. On the other side, the BGM gives an account of the experiments almost in the whole velocity range. Its calculation involves a high degree of computing, and its extension to high \(Z\) seems to be quite complicated. High projectile charges and small-velocity impacts are still an unsolved problem.

Impulsed by hadron therapy to deal with cancer, theoreticians are forced to deal with ionization of DNA molecules by charged projectiles such as \(C^6^+\). Therefore, the challenge of dealing with large \(Z\) has resurfaced, but now within the more complex field of molecular targets. To deal with this challenge, some models reduce the problem to a sum of ionization cross sections of the atoms composing the molecules \([4]\). More refined approaches also take into account the geometry of the molecule, but still the problem of dealing with high \(Z\) persists. Recently Kirchner and collaborators \([5]\) designed a method...
to extrapolate the BGM from $Z = 4$ to tackle the problem of ionization of uracil by $C^6^+$ because the BGM becomes complicated as $Z$ increases.

Some scalings have already been designed to deal with this problem, proposing a normalization of the velocity $v$ and cross section $\sigma(Z, v)$ with $Z$ trying to unveil an universal curve which permits extrapolation to high $Z$. Based on the first Born approximation, a family of scalings is possible, by writing

$$\frac{\sigma(Z, v)}{Z^\alpha} \propto \frac{Z^{2-\alpha}}{v^2} = \left(\frac{Z^{1-\alpha}/v}{\xi}\right)^2 = \frac{1}{\xi^2},$$

(1)

where we can identify different options, for example

$$\begin{align*}
\alpha &= 2, \quad \xi_B = v, \quad \text{Born}, \\
\alpha &= 1, \quad \xi_{JP} = \frac{v}{\sqrt{Z}}, \quad \text{Janey and Presnyakov, reference [6],} \\
\alpha &= 4/3, \quad \xi_M = \frac{Z^{1/3}}{v}, \quad \text{reference [7],} \\
\alpha &= 1.2, \quad \xi_{Mol} = \frac{v}{Z^{1/3}}, \quad \text{for molecules reference [4].}
\end{align*}$$

(2)

The range of validity of a given theoretical method is generally expressed in terms of the corresponding $\xi$. It is well known that the Born scaling holds when the Sommerfeld parameter is small, i.e. $\xi_B = v \gg Z$. The most popular scaling at intermediate impact energies is that of Janey and Presnyakov using $\xi_{JP}$ [6]. It was originally introduced to deal with dipole transitions, but today it has been extended to a large variety of inelastic direct processes with great success. We will prove that the CDW strongly relates to this scaling. There are also other scalings: $\xi_M$ proposed by Montenegro et al [7], which work better at lower velocities, while Gillespie has also devised a scaled exponential universal factor with the argument $\xi_{JP}$ [8]. A comprehensive study of the different expressions and approaches was published by Kaganovich et al [9].

In this article we examine the ionization of simple atoms, hydrogen and helium, by the impact of high charges. By high charges we mean $Z$ as large as 30 for hydrogen and 56 for helium. Our strategy is novel and creative. We propose that the ionization cross section can be expressed in terms of a particular Padé approximation, which is essentially a coefficient of polynomials in terms of the velocity $v$. The zeros of the one in the denominator correspond to the poles of the cross section in the complex plane of the velocity. We find that these poles in the CDW theory move with $Z$ following a certain pattern to the point that we can find an approximated closed form for large $Z$, which we find is related to the Janey and Presnyakov parameter $\xi_{JP}$. We reduce the problem to just two moving poles in the upper complex plane and their conjugates in the lower one, determining the cross section in terms of the $v$ and $Z$. At the very end, the ultimate challenge of this strategy is the description of the experimental cross sections. We find that for protons, antiprotons and He$^{++}$ impact, the experimental data can be very well replicated with four poles in the whole energy range. Inner-shell ionization can also be described with four poles as well as O$^{++}$ on helium. In conclusion, this article proposes that the ionization cross section can be reduced to the knowledge of the positions of the four poles in the velocity complex plane.

The idea that the ionization cross section could have poles in the velocity complex plane should not be peculiar: Green operators have poles in the imaginary component in the k-space, and resonances are explained in terms of poles in the energy complex plane. In a similar manner the maximum of the ionization cross section is here read as the presence of a pole near to the real axis.

The work is organized as follows. After introducing the Padé approximant in section 2, we proceed to find the poles of the Born and CDW theoretical methods. And finally we localize the position of the poles projected by the experimental data. Atomic units are used.

2. Theory

2.1. Experimental and numerical data set

We should first define our Universe of work, which is the target of our study. In table 1 we resume an experimental data set (EDS) of single ionization cross sections $\sigma^{\text{exp}}(Z, v)$ from different laboratories totalling 125 (203) experimental values for hydrogen (helium) for different charges $Z$ and impact velocities $v$, including antiproton impact ($Z = 1$). Details of the references as well as the charges and velocities considered are displayed in table 1. There are some other experiments on the impact of projectiles that cannot be considered as required by the theory. This table should not be considered completely; we simply present the most relevant ones obtained in a more or less systematic way. To have an idea of the measurement spectrum, in figures 1(a) and 2(a) we show each experimental value in a $Z - v$ plot for hydrogen and helium, respectively. Helium, for obvious reasons, presents a more complete panorama.

The only theory that we use in this article is the CDW. In a similar manner we build a numerical data set (NDS) of 245 (198) values of net (or gross) ionization cross sections of hydrogen (helium) by the impact of different $Z$ and $v$. In figures 1(c) and 2(c), we show each theoretical calculation in the $Z - v$ plot for hydrogen (helium). Some values can be found in the literature: for hydrogen in [28] and for helium in [29] for charges $Z = 1$ to 8. We also extended the calculation for negative charges up to $Z = -8$ ($Z = -4$) for hydrogen (helium). Of course, except for antiprotons, negative charges are unrealistic, but let us understand the process in a wider range.

Before proceeding we point out that for the helium target, we did a full calculation of its continuum state expanding in spherical harmonics of the potential obtained with the depurated inversion model [30]. This potential reads

$$V_{\text{He}}(r) = -\frac{1.0764}{r} \exp(-2.79681r)(1 + 0.62529r) + \frac{0.0764}{r} \exp(-18.3544r)(1 + 9.8617r) - \frac{1}{r},$$

(3)
Table 1. The EDS. Projectile energy ranges are in KeV/amu and $N$ is the number of points.

| Target | $Z$ | Reference Energy range | $N$ | Target | $Z$ | Reference Energy range | $N$ |
|--------|-----|------------------------|-----|--------|-----|------------------------|-----|
| $H^-$  | 1   | 31–800                 | 19  | He     | 3   | 640–2310               | 3   |
| $H^+$  | 1   | 30–1500                | 11  | He     | 4   | 190–2310               | 6   |
| $H^+$  | 1   | 9–75                   | 12  | He     | 5   | 190–2440               | 4   |
| $H^+$  | 1   | 38–1500                | 27  | He     | 6   | 640–2260               | 3   |
| $H^+$  | 2   | 31–550                 | 17  | He     | 7   | 1440–2260              | 2   |
| $H^+$  | 2   | 19–64                  | 12  | He     | 8   | 640–2260               | 4   |
| $H^+$  | 3   | 57–387                 | 14  | He     | 24–54 | 3600 | 8 |
| $H_{2/2}^+$  | 11  | 1100                   | 8   | He     | 6–44 | 22 | 1400 | 7 |
| $H_{2/2}^-  $ | 1   | 13–29                  | 5   | He     | 26–44 | 23 | 1000 | 10 |
| $He$    | 1   | 40–2890                | 26  | He  | 22–37 | 23 | 500 | 10 |
| $He$    | 1   | 13–500                 | 23  | He  | 9–31 | 23 | 250 | 23 |
| $He$    | 1   | 64–2380                | 17  | He  | 5–16 | 23 | 100 | 8 |
| $He$    | 1   | 15–5000                | 16  | He  | 8 | 24 | 27–72 | 1 |
| $He$    | 2   | 50–1585                | 16  | He  | 6 | 25 | 310–1140 | 20 |
| $He$    | 2   | 640–2310               | 3   | He  | 10–14 | 26 | 1050 | 5 |
| $He$    | 3   | 50–390                 | 11  | He  | 6,8 | 27 | 70–250 | 15 |

Figure 1. Hydrogen target. (a) EDS in a $Z$–$v$ diagram as resumed in table 1; solid line: $v_{\text{max}} = \sqrt{v_B^{\text{max}}^2 + c_1 Z}$, as given by equation (5). (c) NDS in a $Z$–$v$ diagram; solid line: position of the maximum as in panel (a). (b) The relative error of the CDW values versus the experiments, as defined in equation (8) in terms of $v/v_{\text{max}}$. (d) The relative error of $\sigma$ [4,4] versus the CDW values, as defined in equation (22) in terms of $v/v_{\text{max}}$.

warranting at least four significant figures of the binding energy, and three figures for the mean values of $\langle 1/r \rangle$, $\langle r \rangle$ and $\langle r^2 \rangle$ as compared with Hartree Fock. In general, errors in the CDW numerical calculations can be estimated around 2% or perhaps a little more [29].

2.2. Definition of the validity regime

From our NDS we can easily obtain the velocity $v_{\text{max}}$ where the cross section is maximum, i.e.

$$\sigma_{\text{max}}(Z) = \sigma(Z, v_{\text{max}}(Z)).$$ (4)
Figure 2. Helium target. (a) EDS in a $Z - v$ diagram as resumed in table 1; solid line: $v_{\text{max}} = \sqrt{v_{\text{max}}^2 + c_1 Z}$, as given by equation (5). (b) NDS in a $Z - v$ diagram; solid line: position of the maximum as in panel (a). (c) The relative error of the CDW values versus the experiments, as defined in equation (8) in terms of $v/v_{\text{max}}$. (d) The relative error of $\sigma_{[4,4]}$ versus the CDW values, as defined in equation (22) in terms of $v/v_{\text{max}}$.

In figures 3(a) and (b) we show the values of $v_{\text{max}}^2(Z)$ and $\sigma_{\text{max}}(Z)$ for hydrogen (helium). Notably for $Z > 0$, $\sigma_{\text{max}}(Z)$ and $v_{\text{max}}^2(Z)$ behave linearly with $Z$, and the dependence can be fitted approximately as

$$v_{\text{max}}^2 \approx (v_{\text{max}}^B)^2 + c_1 Z \quad \rightarrow c_1 Z, \quad \text{and},$$

$$\sigma_{\text{max}} \approx \frac{Z^2 \sigma_{\text{max}}^B}{1 - c_2 \sqrt{Z + Z^\text{max}^c_3 \rightarrow c_3 Z}},$$

where $v_{\text{max}}^B = 1(1.5)$ is the velocity where the Born approximation $\sigma_B$ is maximum for hydrogen (helium), and $Z^2 \sigma_{\text{max}}^B$ is the value of the Born cross section at the maximum with $\sigma_{\text{max}}^B = \sigma_B(v_{\text{max}}^B) = 7.63 (3.67)$ for hydrogen (helium). The rest of the coefficients are found to be: $c_1 = 1(1.59)$, $c_2 = 0.48(0.54)$ and $c_3 = 7.32(5.42)$ for hydrogen (helium). Note that $c_1$ is equal or close to the mean velocity of the electron in the initial state, indicating that the Janev and Presnyakov variable could be generalized as $v/\sqrt{c_1 Z}$. Relation (5) is fundamental in this article, since it lets us introduce a criterion to define the validity of the CDW theory, and that is when

$$v \lesssim v_{\text{max}}, \quad \text{or} \quad \xi_{\text{JP}} \lesssim \sqrt{c_1 + 1/Z(v_{\text{max}}^B)^2} \rightarrow \sqrt{c_1},$$

which is stated in terms of the parameter Janev and Presnyakov $\xi_{\text{JP}}$ and not to the Sommerfeld criterion defined as $\xi_B = v \gg Z$. It is important to note that negative charges also have a linear dependence with $Z$ but with a different slope. The magnitude $v_{\text{max}}$, as defined in equation (5), is displayed in the solid line in figure 1(a) for hydrogen and figure 1(b) for helium to indicate the intermediate energy region or the maximum of the cross section.

Now we can quantify the validity of the CDW by contrasting this theoretical prediction with the experiments in terms of $v/v_{\text{max}}$. In figures 1(b) and 2(b) we display the relative error defined as

$$e_{\text{CDW-\exp}}(\%) = \frac{\sigma_{\text{CDW}}(Z, v) - \sigma_{\text{exp}}(Z, v)}{\sigma_{\text{exp}}(Z, v)} \times 100,$$

for all the Universe of experiments listed in table 1 (or shown in figure 1(a) for hydrogen and figure 1(b) for helium), where we can observe that the range of applicability of the CDW is indeed restrained to $v \gtrsim v_{\text{max}}$. From the figures, we can state that the CDW predicts the experiments with $\pm 20\%$ at $v \sim v_{\text{max}}$, converging for larger $v$. At the same time the error explodes for $v < v_{\text{max}}$. Therefore, $v_{\text{max}}$, as defined in equation (5), rests as a firm standpoint of the intermediate energy.
2.3. The Padé approximant

First we divert the atomic ionization cross section \( \sigma(Z, v) \) with the help of the diagonal Padé approximant \( P_{m,m} \) and the asymptotic limit \( L(v) \) by writing

\[
\sigma_Z^{[m,m]}(Z, v) = Z^2 L(v) P_{m,m}(Z, v), \tag{9}
\]

\[
P_{m,m}(Z, v) = \sum_{\mu=0}^{m} \frac{n_{\mu}(Z)v^\mu}{\sum_{\mu=0}^{m} d_{\mu}(Z)v^\mu}, \tag{10}
\]

\[
L(v) = \frac{A}{v^2} \log(1 + Bu^2), \tag{11}
\]

with \( Z^2 L(Z, v) \) being the correct asymptotic limit, and therefore it is required that

\[
\lim_{v \to \infty} P_{m,m}(Z, v) = 1. \tag{12}
\]

Written in this way \( L(Z, v) \) is finite at the origin: \( L(v) \to AB \), as \( v \to 0 \). After a series of trials we have considered convenient to use the following contracted form for the diagonal \( P_{2n,2n} \) approximant

\[
P_{2n,2n}(Z, v) = \prod_{j=1}^{n} \frac{v^2}{(v - v_j)(v - v_{-j})}, \tag{13}
\]

where \( v_{\pm j} \) are the position of the poles in the velocity complex plane defined as

\[
v_{\pm j} = v_{jr} \pm iv_{ji}. \tag{14}
\]

We cast on the real and imaginary components of the poles, \( v_{jr} \) and \( v_{ji} \), the dependence on the projectile charge \( Z \); that is we expect: \( v_j(r_1) = v_{jr}(Z) \). All the information is then being reduced to the position of \( n \) poles in the complex upper plane of the projectile velocity: \( v_{jr} > 0 \), and their conjugate in the lower plane, \( -v_{ji} < 0 \). The imaginary parts warrant that there is no divergence at real velocities, and this is the reason why we have chosen the particular expression given by (13). By construction the term \( P_{2n,2n} \) satisfies the condition (12), and at the threshold it behaves as \( v^{2n} \), i.e.

\[
\sigma^{[2n,2n]}(Z, v) \to Z^2 AB v^{2n} \prod_{j=1}^{n} \frac{1}{|v_j|^2}. \tag{15}
\]

We must now find the best value of \( n \) that determines the degree of the Padé approximant to be used. The problem is that there is no solid knowledge about the actual behavior of the ionization cross section in this region. In the literature we find different extrapolated expressions, contradictory to each other, showing a certain level of uncertainty. Just to illustrate the spread: the recommended values of Rudd [11] behave as \( v^{2\eta} \) with \( D = 0.907(1.52) \) for hydrogen (helium), but the successful expression of Gillespie decays exponentially [8].

One illuminating study is the theory of inner-shell ionization developed in the 1970s by Basbas et al [31], which has

Figure 3. (a) Hydrogen target. Solid lines: \( v_{max}^2 \) and \( \sigma_{max} \) as a function of the projectile charge \( Z \), as defined in equations (5) and (6), respectively; empty circles: the corresponding CDW results. (b) Similar to panel (a) for helium. (c) Hydrogen target. Empty circles: values of the imaginary parts of the poles \( v_1r \) and \( v_2r \) obtained with the CDW results; solid lines: fitted closed forms \( V_1r \) and \( V_2r \) as given by equation (23). (d) Similar to panel (c) for helium. (e) Hydrogen target. Empty circles: values of the imaginary parts of the poles \( v_{1i} \) and \( v_{2i} \) obtained with the CDW results; solid lines: fitted closed forms \( V_{1i} \) and \( V_{2i} \) given by equation (23). (f) Similar to panel (e) for helium.
largely been used with great effectiveness. This theory is based on the simple first Born that the authors found to have a behavior \( v^8 \) in the region where \( v \ll v_{\text{max}} \), which is the region that we precisely need to access. Inspired by this, we propose \( n = 4 \) leading to a \( P_{88} \) that is

\[
\sigma^{[8,8]}(Z, v) = Z^2 L(v) P_{8,8}(Z, v),
\]

which can be seen as a simple product of two \( P_{44} \), or a product of four \( P_{22} \). In this way we expect our expression to be high- and low-energy properly bonded.

In the next two subsections of this article we will concentrate on finding the poles of the Born and CDW theories, which we expect to be valid for \( v \gtrsim v_{\text{max}} \). In that case we resume the calculation with the use of just \( P_{44} \) having the correct high-energy bond, and \( v^8 \)-behavior at the origin. This is supposed to be incorrect, but it is worthwhile to include more poles to refine the expression in a region where the CDW fails. We will find that \( \sigma^{[4,4]}(Z, v) \) is enough, and we reserved \( \sigma^{[8,8]}(Z, v) \) to investigate the experimental data, which is a much more demanding task. We can also read \( \sigma^{[4,4]}(Z, v) \) as a particular case of \( \sigma^{[8,8]}(Z, v) \), namely

\[
\sigma^{[4,4]}(Z, v|v_1, v_2) = \sigma^{[8,8]}(Z, v|v_1, v_2, v_3 = 0, v_4 = 0). \tag{17}
\]

Thus, we can then identify the two extra poles commanding the intermediate and the threshold. By threshold we mean the region starting from a few keV, where the projectile can be considered a heavy particle describing a straight line trajectory.

2.4. The Born poles

The first test to check that our expression is appropriate is to examine the first Born approximation, which is supposed to be correct as \( Z \to 0 \). Further, the Born approximation lets us determine the values of \( A \) and \( B \) of the asymptotic limit expression \( L(Z, v) \). Thus, we obtain \( A = 3.52(6.11) \), and \( B = 62.1(3.22) \) for hydrogen (helium). The values of \( A \) agree with those used by [11, 32, 33]. While dealing with \( \sigma^{[4,4]}(0, v) \) we have observed that \( v_{1r} \) was positive while \( v_{2r} \) was always negative and \( v_{2r} \sim -v_{1r} \). So we decided to set

\[
v_{2r} = -v_{1r}, \tag{18}
\]

and reduce the number of free parameters to be fitted to three. We will come back to this point. The values of \( v_{1r}, v_{1i} \) and \( v_{2r} \), displayed in table 2 in the row corresponding to \( Z = 0 \) for hydrogen and helium targets, as indicated. This table also displays the poles corresponding to \( \sigma^{[8,8]}(0, v) \) using the same data set and also imposing \( v_4 = -v_3 \). At intermediate energies the results are very similar, but at lower velocities they differ: \( \sigma^{[4,4]} \propto v^8 \), while \( \sigma^{[8,8]} \propto v^{10} \).

2.5. The CDW–EIS poles

Next, we proceed to find the values of the poles \( v_1 \) and \( v_2 \) governing the CDW theory. For this we use the NDS shown in figures 1(a) and 2(a). As in the Born approximation, we considered \( v_{2r} = -v_{1r} \); the agreement with the numerical data is not altered substantially if we let them vary freely. One interesting feature of the Padé approximant so-defined is that the sum of the residues of all the poles of the boundary-corrected function \( Q_{44}(v) = P_{4,4}(v) - 1 \) is

\[
S_{4,4} = \sum_{j=1}^{2} \left( \text{Residue}[Q_{44}]_{|v_j} + \text{Residue}[Q_{44}]_{|v_j} \right)
= 2(v_{1r} + v_{2r}), \tag{19}
\]

so by setting condition (18) then \( S_{4,4} = 0 \). As a consequence of this, the integration on a closed curve \( C = |v| \to \infty \) also produces a null value

\[
I_{4,4} = \int_{|v| = \infty} Q_{44}(v) \, dv = 0. \tag{20}
\]

Another way to visualize equation (20) is to expand \( Q_{44} \) for large values of the complex magnitude \( v \) to give

\[
Q_{44}(v) \to \frac{2(v_{1r} + v_{2r})}{v} + O \left( \frac{1}{v^2} \right), \tag{21}
\]

by setting \( v_{1r} + v_{2r} = 0 \), we obtain null circulation given by equation (20). If we require \( \sigma^{[2n,2n]}(Z, v) \to Z^2 L(v) \) as the real magnitude \( v \to \infty \), we are restraining the limit to just the real axes, but the condition (18) generalizes this limit in the entire velocity complex velocity magnitude \( |v| \to \infty \).

In figures 3(c) and (d), we plot the values of \( v_{1r} \) and \( v_{2r} \) for hydrogen (helium), and in figures 3(e) and (f) the values of \( v_{1i} \) and \( v_{2i} \) for hydrogen (helium) as a function of the impinging charge \( Z \). We have observed that the prediction of the Padé \( P_{4,4} \) approximant is excellent in our range of interest here. To illustrate that our Padé approximant \( \sigma^{[4,4]} \) gives a quite precise description of the CDW results, in figure 1(d) we plot the relative errors with respect to the full numerical results \( \sigma^{\text{CDW}} \) defined as

\[
e^{-[4,4] - \text{CDW}} = \frac{\sigma^{[4,4]}(Z, v) - \sigma^{\text{CDW}}(Z, v)}{\sigma^{\text{CDW}}(Z, v)} \times 100, \tag{22}
\]

as a function of \( v/v_{\text{max}} \) for all the cases of the NDS. For \( v/v_{\text{max}} \gtrsim 1 \), the errors are less than \( 4\% \), but most of them are around or even less than \( 2\% \), which is of the order of the numerical uncertainties of the \( \sigma^{\text{CDW}} \) calculation. Similarly, in figure 2(d) we show the equivalent relative error for helium. The agreement of \( \sigma^{[4,4]} \) with the numerical results covers almost all the velocity range of our interest, except at the threshold \( v \ll v_{\text{max}} \), where the \( v^4 \)-dependence imposed by our \( P_{4,4} \) is no longer correct.

There are a lot of interesting rules in the position of the poles which can lead to some physical interpretation. The first observation, which is perhaps the main finding of this work, is that the components of the poles \( v_{1r}, v_{1i} \) and \( v_{2r} \) obey certain patterns to the point that we can find a reasonably fitted closed
form, say $V_{1r}, V_{1i}$ and $V_{2i}$, expressed as

$$
\begin{align*}
V_{1r}(Z) &= -V_{2r}(Z) \approx k_1 \sqrt{k_2 + Z} \rightarrow k_1 \sqrt{Z} \\
V_{1i}(Z) &\approx k_3 \sqrt{k_4 + Z} \rightarrow k_3 \sqrt{Z} \\
V_{2i}(Z) &\approx k_5 \sqrt{(k_6 + Z)^{1/2}} \rightarrow k_5 Z^{1/4} \sqrt{Z}
\end{align*}
$$

(23)

where $k_1 = 0.57(0.53), k_2 = 0.97(4.18), k_3 = 0.57(0.64), k_4 = 2.3(2.8), k_5 = 0.91(1.1)$ and $k_6 = 0.28(0.0)$ for the hydrogen (helium) target. The fact that $\text{Im}[V_{\pm 2}(Z)] = 0$ does not present any problems, since the divergence occurs at negative (unphysical) impact velocities. For negative charges, $-\infty < Z < 0$, we can also fit the NDS better and the pole description is very good and the errors are small; this is probably because capture is absent, the process of ionization becomes simpler and the poles are enough to describe the mechanism in a cleaner way.

The poles can now be visualized at the approximate positions

$$
V_{\pm j}(Z) = V_j \pm iV_j, \quad j = 1, 2,
$$

(24)

and, in this way, we can obtain an approximate ionization cross section $\sigma^{[4]}(Z, v)$ defined through equation (13) with the poles at $V_1$ and $V_2$ instead of $v_1$ and $v_2$, respectively. What is interesting is that $\sigma^{[4]}(Z, v)$ has a closed form and it will let us extract valuable information.

We now raise the question to what extent does the CDW verify the Janev and Presnyakov scaling. It is convenient to scale $\sigma^{[4]}(Z, v)$ as follows

$$
\sigma^{[4]}_{\text{JP}} = \frac{1}{ZA \log(1 + Bv^2)} \frac{Z v^2}{|v - v_1|^2 |v - V_2|^2}
$$

(25)

or in terms of $\xi_{\text{JP}}$, it reads

$$
\sigma^{[4]}_{\text{JP}} = \frac{\xi_{\text{JP}}^2}{\xi_{\text{JP}} - \frac{v_1}{v}} \left| \frac{\xi_{\text{JP}} - v}{v} \right|^2.
$$

(26)

In figure 4 we plot $\sigma^{[4]}_{\text{JP}}$ in solid lines compared with the full-numerical CDW counterpart denoted by empty circles. The agreement is quite good for $\xi_{\text{JP}} \gtrsim 1$, indicating that the pole representation is reliable. For large values of $Z$ (i.e. $Z > \max(k_2, k_4, k_6)$) it behaves as

$$
\sigma^{[4]}_{\text{JP}} \rightarrow \frac{\xi_{\text{JP}}^2}{|\xi_{\text{JP}} - k_1 + ik_3|^{1/2} |\xi_{\text{JP}} + k_1 + ik_3 Z^{1/4}|^{1/2}},
$$

(27)

and this is almost the Janev and Presnyakov scaling, except for the imaginary part of the second pole behaving as $Z^{1/4}$. It breaks a perfect scaling with $\xi_{\text{JP}}$, and it plays an important role for very large values of $Z$. In our analysis the variable $\xi_{\text{JP}}$ comes up in natural form as a consequence of the particular movements of the poles in the complex plane. The poles mold the cross section around $\xi_{\text{JP}} \gtrsim k_1$, that is precisely the region where this scaling was originally intended to work at by Janev and Presnyakov in its original paper [6].

2.6. The experimental poles

By observing the excellent performance of the Padé approximant, we are encouraged to extend this scheme to reproduce

| $Z$       | Target | $v_{1r}$ | $v_{1i}$ | $v_{2r}$ | $v_{2i}$ | $v_{4r}$ | $v_{4i}$ |
|-----------|--------|----------|----------|----------|----------|----------|----------|
| -1        | H      | 0.5869   | 1.213    | 0.4573   | 0.4545   | 0        | 0        |
| (Born) 0  | H      | 0.560    | 0.7645   | 0.352    | 0        | 0        | 0        |
| (Born) 0  | H      | 0.5013   | 0.7873   | 0.2763   | 0.3117   | 0        | 0        |
| 1         | H      | 1.1336   | 1.304    | 0.9053   | 0.6008   | 0        | 0        |
| 2         | H      | 0.4715   | 1.920    | 0.147    | 0.5287   | 0        | 0        |
| -1        | He     | 0.7558   | 1.673    | 0.6787   | 0.3120   | 0        | 0        |
| (Born) 0  | He     | 0.5417   | 0.8020   | 1.387    | 0        | 0        | 0        |
| (Born) 0  | He     | 0.7367   | 1.024    | 0.3021   | 0.2214   | 0        | 0        |
| 1         | He     | 1.207    | 1.273    | 0.5744   | 0.3449   | 0        | 0        |
| 2         | He     | 1.051    | 2.053    | 1.357    | 0.8662   | 0        | 0        |
Figure 5. The ionization cross section of hydrogen, helium and the K-shell of neon as a function of the projectile velocity by the impact of different projectiles as indicated. Theory: red solid line $\sigma^{[8,8]}$, and symbols are the experiments.

the experiments to the the best that our model permits. In this case we need to accede to small velocities: i.e. $v < v_{\text{max}}$ that we have discarded when describing the theory valid for $v \gtrsim v_{\text{max}}$. In that case the $P_{44}$ was enough. But here we pretend our expression covers all the experimental range and, therefore, we must resort to the original $P_{8,8}$, which we suppose is more appropriate.

The great problem is that the experimental data are very limited. Even for the most popular systems the measurements are very sparse. A direct fitting of the data is possible for few cases, such as $H^+$ and $He^{++}$ impact, most of them carried out by Shah, Gilbody, Knudsen and collaborators. For antiproton impact on hydrogen the fitting can be possible by resorting to the Havlplund et al measurements on molecular hydrogen divided by 2 [17] to obtain some values for $v < v_{\text{max}}$. In this way we have a minimum number of pivots to use the minimization algorithm. Besides, the spread of the experimental errors introduce some noise in the fitting procedure. To guide the algorithm we have sometimes needed to introduce some theoretical values at very large impact velocity in the region where there is no experiment at all, but the theory is expected to hold.

The expression $\sigma^{[8,8]}(Z, v)$ depends in principle on eight variables corresponding to the real and imaginary part of the four poles in the upper plane; we follow the same conditions of equation (18) and impose

$$v_2^r = -v_1^r, \quad v_4^r = -v_3^r, \quad (28)$$

reducing the problem to six parameters. In a similar manner to equations (19) and (20), the condition (28) produces $S_{88} = I_{88} = 0$.

We were able to fit just three experimental cases: $p^-$, $H^+$ and $He^{++}$ on hydrogen and helium, as shown in figures 5(a)–(f). Calculations based on $P_{8,8}$ give very good agreement with the experiments. Stimulated by this performance we go further facing the system $Li^+$ and $O^+$ on helium, where we can put together a reasonable set of experimental values for the fitting procedure to work. As shown in figures 5(g) and (h), the agreement is excellent even for $v \ll v_{\text{max}}$ where the capture channel plays the dominant role. The Padé $P_{8,8}$ can also apply to the inner shell, as shown in...
figure 5(i), where we fit the experiments of ionization of the inner shell of neon [34–36]. The agreement is again excellent. And we tested this performance for other inner shell cases as well.

Inspecting the values of components of the poles in table 2 we find notable behavior, for example, in some cases \( v_{2y} = v_{4z} = 0 \) along with the condition (28) constraining the problem to find just four parameters. Recall that the fact that the imaginary part is null does not present any problems since the divergence occurs at negative (unphysical) impact velocities.

3. Summary

We have studied the single ionization of a punctual Coulomb charge on hydrogen and helium. To deal with impact velocities \( v > v_{\text{max}} \), we have proposed that the cross section can be separated in an asymptotic dependence times a Padé \( P_{44} \) written in terms of our poles: two in the upper velocity complex plane and their conjugates in the lower plane. By setting condition (18) we could find the components of the poles for an NDS consisting of 443 numerical CDW full calculations for different values of \( Z \). The agreement was estimated less than 4% for \( v > v_{\text{max}} \). Finally, we deal with the experimental data by using an appropriate Padé \( P_{88} \) instead. For the few experiments available that we could fit, we have found very good agreement with the data.

In this article we study the poles in the velocity complex plane by considering the projectile charge as a parameter; in an upcoming article [37] we describe the poles in the charge complex plane by considering the velocity as a parameter. The reduction of the physics of the problem to find the poles in the complex plane is appealing. Finding the logic of these reduction of the physics of the problem to find the poles in the complex plane by considering the velocity as a parameter. The agreement with the data was established less than 4%.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

J E Miraglia https://orcid.org/0000-0002-7876-0283

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