Soft-electron emission peak in ion-helium collisions

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We study the angular distribution of electrons, emitted in ion-helium collisions, with low velocities relative to the target. We use an expansion of the ionization doubly differential cross section, in Legendre polynomials, with electron velocity-dependent weight coefficients that define the angular shape of the distribution. We determine these coefficients from available experimental data for H^+, He^{2+}, C^{6+}, and O^{8+} projectiles at 1- and 1.84-MeV impact energies, and we evaluate them by using the first Born and the continuum-distorted-wave–eikonal-initial-state (CDW-EIS) approximations. The experimental results and CDW-EIS calculations confirm the existence of forward-backward asymmetry in the soft-electron emission peak. We discuss the dependence of theoretical and experimental parameters on the impact energy and the charge of the projectile.

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I. INTRODUCTION

Emitted electron spectra from ion-atom collisions at high and intermediate energies show three characteristic features, i.e., binary electrons (BE's), electrons captured to the continuum of the projectile (ECC), and soft electrons (SE's). These features are identified as enhancements of the electron emission in particular regions of the spectra. A great deal of measurements and theoretical descriptions have been devoted to the study of the BE and ECC effects and their dependence on the target, impact energy, and projectile charge [1]. The SE's show up as a high yield of electrons emitted with low velocity relative to the target ($\mathbf{v}$), growing up towards a maximum value at $v=0$, the so-called soft-electron peak (SEP). Little attention has been payed to the study of the SEP, due mainly to the experimental difficulties involved in the accurate measurement of slow electrons. Theoretical studies of the SEP have been limited mainly to the first Born approximation (FBA) [2,3]. This approach gives, at the limit $v \to 0$, a $1/v$ divergence in the cross section $d\sigma/d\mathbf{v}$, doubly differential in the direction and modulus of $\mathbf{v}$ (DDCS). This divergence originates from the normalization factor of the Coulomb wave function describing the outgoing electron and has forward-backward symmetry in the direction of the incident projectile velocity. Otherwise, the SE production mechanism can be thought of as excitation of the electron to the low-lying continuum of the target atom, and this idea has allowed the continuation of the ion-atom excitation density-matrix formalism to the ionization threshold [4–6]. This is achieved by writing the cross section as a Legendre polynomial expansion with coefficients related to the density-matrix elements. The extrapolation of these coefficients for high excited levels predicts an asymmetry for the SEP in the $v \to 0$ limit [7]. This method has been applied to the description of the ECC and electron-loss peaks [2,8]. Recently, Suarez *et al.* [9] have presented an experimental study of the shape of the SEP, in the collision of 100-keV/amu H^+ and He^{2+} projectiles on Ne atoms. They have found experimental evidence of a strong asymmetry in the SEP and have given values for the abovementioned coefficients. However, the relatively low impact energy and the many-electron target atom considered complicate a possible comparison with current distorted wave methods. In this work we consider available experimental data of the DDCS for ion-helium collisions at high impact energies [10]. We determine the experimental asymmetry parameters, which are compared with theoretical values calculated using the Born approximation and the continuum-distorted-wave–eikonal-initial-state method (CDW-EIS) [11]. These results allow for a study of the dependence of the parameters on the energy and charge of the projectile.

II. THEORETICAL CALCULATIONS

We introduce an angular expansion for the DDCS for ionization, differential in energy E and direction Ω of the emitted electron. The problem has cylindrical symmetry around the projectile direction, and the expansion can be made in terms of Legendre polynomials:

$$\frac{d^2\sigma}{dE\,d\Omega}=\sum_l \beta_l(i,V,v)P_l(\cos\vartheta)\ , \tag{1}$$

where ϑ is the angle between the emitted electron and the incident ion directions. The coefficients β_l depend, in principle, on the initial electronic state i, the electron velocity v, and the velocity V and charge Z of the incident ion. This expansion has been formerly proposed for the analysis of the ECC cusp to obtain an apparatus-independent comparison of different measurements [8]. In this case the coefficients β_l were assumed to be analytical functions of v and the DDCS was written as

$$\frac{d^2\sigma}{dE\,d\Omega}=\sum_l \sum_k \beta_l^k v^k P_l(\cos\vartheta)\ . \tag{2}$$

The coefficients in Eq. (2) have been extrapolated below the ionization threshold by Burgdörfer [4], Schöller, Briggs, and Dreizler [5], and Rodriguez and Miraglia [6], and evaluated for electronic excitation processes in ion-hydrogen collisions. They make a partial-wave decomposition of the continuum final state, to express the DDCS for ionization, and hence the asymmetry parameters, in terms of density-matrix elements for continuum excitation. These elements are related to those for bound states by continuity across the ionization threshold, allowing for the evaluation of the parameters β_l for excitation processes.

Factoring out the angle-independent factor, we can write Eq. (1) as

$$\frac{d^2\sigma}{dE\,d\Omega}=\beta_0(i,V,v)\left[1+\sum_l \alpha_l(iV,v)P_l(\cos\vartheta)\right], \quad (3)$$

where $\beta_0(i,V,v)$ is proportional to the singly differential cross section (SDCS) and α_l are the *relative asymmetry parameters* (RAP's) defined as the ratio β_l/β_0. For target excitation to high bound levels, the RAP's are related to the multipoles of the Runge-Lenz vector, and, in particular, α_1 is related to the dipole moment of the remainder excited atom [4].

A similar parametrization has been widely used in photoionization theory [12]. When the electric dipole approximation is used for the transition matrix, the angular distribution of photoelectrons from the (nl)th subshell emitted by unpolarized radiation is given by

$$\frac{d\sigma_{nl}(\varepsilon)}{d\Omega}=\frac{\sigma_{nl}(\varepsilon)}{4\pi}\left[1-\tfrac{1}{2}B_{nl}(\varepsilon)P_2(\cos\vartheta)\right], \quad (4)$$

where ε is the photon energy and ϑ is the angle between the incident photon beam and the photoelectron direction. In this case the velocity of the emitted electron is determined by ε and the bound energy of the initial state. The asymmetry coefficient $\beta_{nl}(\varepsilon)$ has become a standard description parameter which provides information concerning both dipole transition-matrix elements and interferences between allowed final states. We note that in this case we have no post-collisional electron-projectile interaction able to produce polarization on the final continuum state, and the contribution of the P_1 polynomial is zero.

The first Born approximation (FBA) is usually employed when dealing with fast ion-atom collisions, specially in the region where small momentum transfer is expected to dominate, i.e., excitation and slow electron emission. For a 1s initial state and a Coulomb final wave for the emitted electron, Eq. (1) can be written in the FBA as the double series in Eq. (2) with the constraint that $\beta_l^k(i,V)=0$ for $k+1$ odd and for $l>k+2$ [13]. For a general hydrogenic initial state, with principal quantum number n, Burgdörfer *et al.* [14] found, in the limit of $v\rightarrow 0$,

$$\frac{d\sigma}{dE\,d\Omega}=\sum_{l=0}^{2n}\beta_l(i,V,v\rightarrow 0)P_l(\cos\vartheta), \quad (5)$$

with even l_0. Therefore, for a 1s state and $v\rightarrow 0$, only β_l with $l=0$ and 2 contribute and the SEP has forward-backward symmetry. However this is true only on the top of the SEP, since as $v\neq 0$, nonzero odd coefficients are possible from Eq. (1). This equation has been successfully applied to the electron loss to the continuum process (ELC), where the remainder target is neutral and can only produce a small distortion to the final electron-projectile Coulomb interaction.

In principle, $\beta_l(i,V,v)$ could be nonanalytic in $v=0$, making the double series in Eq. (2) unjustified. Although both the FBA and CDW-EIS provide analytic parameters, we will use Eq. (3) for the parametrization and then observe the v dependence of the coefficients.

In order to evaluate theoretically β_l, we first calculate the DDCS following usual techniques, i.e., analytical evaluation of the transition amplitude and further numeric integration over momentum transfer. We represent the initial state of the helium target by a Roothaan-Hartree-Fock wave function of 5-Z type [15], and the final continuum state is approximated by a Coulomb wave function with effective charge $Z_T=(-2\varepsilon_i)^{1/2}$. The ε_i is the bound-state energy. Having obtained the DDCS, the asymmetry parameters $\beta_l(v)$ are calculated as follows:

$$\beta_l(v)=\frac{2l+1}{2}\int P_l(\cos\vartheta)\frac{d^2\sigma}{dE\,d\Omega}d\Omega\ . \quad (6)$$

We will denote by β_l^B and β_l^C the parameters derived from the FBA and CDW-EIS, respectively.

III. EXPERIMENTAL PARAMETERS

There is a large quantity of experimental data of the DDCS for ionization corresponding to H^+ collisions against different gaseous targets [16,17]. However, for multicharged ions the available experimental data are scarce. As we are interested in the projectile influence on the SEP shape, it seems clear that the two variables that determine a naked projectile action are its charge and its velocity.

Most suitable measurements for studying this dependence have been accomplished by Pedersen *et al.* [10], who have measured DDCS's for H^+, He^{2+}, C^{6+}, and O^{8+} on helium with impact energies of 1 and 1.84 MeV. Electronic spectra have been recorded for seven emission angles: 20°, 35.5°, 60°, 90°, 118°, 144.5°, and 160°. Electronic energy distribution starts from 1 eV for H^+ and C^{6+} and 6 eV for He^{2+} and O^{8+} [18]. These electron energies correspond to velocities 0.27 and 0.6 a.u., respectively. Even when these velocities are on the wings of the SEP, as projectile velocities are quite high (i.e., 6.33 and 8.58 a.u.), we can suppose that SEP characteristics remain unchanged, with little influence from projectile capture effects. A more serious drawback comes from the reduced number of angular data, in particular for small emission angles. The SEP asymmetry is produced by the electron-projectile interaction and can be considered as a continuation of the two-center ridge, which is observed as a large emission of electrons in the forward direction with velocities comprised between 0 and **V**. This ridge has a broad angular width, which is about 30°, for H^+-He collisions at 100 keV/amu [19]. Therefore, the information for small angles should be very important for a precise determination of the asymmetry. We extract the experimental parameters β_l^E by replacing the expansion given by Eq. (1) by a finite sum:

$$\frac{d^2\sigma}{dE\,d\Omega}=\sum_{l=0}^{N}\beta_l^E(i,V,v)P_l(\cos\vartheta)\ . \tag{7}$$

There is not an *a priori* criterion to determine the best value for N, so we must use some numerical stability criterion. For each value of v we have seven experimental data corresponding to seven emission directions, and consequently we must have $N\leq 5$ for the fit procedure to make sense. On the other hand, FBA predicts $N=2$ in the limit $v\rightarrow 0$. This limits the range to $2\leq N\leq 5$.

We have used a least-squares-fit program that provides $\beta_l^E(v)$ with their respective errors, taking into account the original experimental data errors. The program has been run for each projectile charge Z, projectile velocity V, and electron velocity v in order to fit the respective experimental angular distribution, using $N=2$–5. We found that $\beta_0^E(v)$ and $\beta_1^E(v)$ have relative errors lower than 5% and 15%, respectively, in every case, and that their absolute values remain within the error bounds as N is increased. A similar situation is found for $\beta_2^E(v)$, and $\beta_3^E(v)$ when v is large ($v>1$) except for its relative error, which amounts to 30% in the worst cases. However, at low v the absolute values found for $\beta_2^E(v)$ and $\beta_3^E(v)$ are small, as can be observed in Figs. 3 and 4. In these cases the numerical errors are relatively large, but are small in absolute value, and these coefficients remain stable with N. The $\beta_4^E(v)$ and $\beta_5^E(v)$ have inaccuracies larger than their variation with v, Z, or V; in particular, $\beta_4^E(v)$ do not reach a stable value as N changes. Strong angular oscillations of high-order Legendre polynomials make the respective coefficients numerically unstable, and they could only be determined when detailed angular distributions are available. We conclude that only β_0^E, β_1^E, β_2^E, and β_3^E may be considered reliable, and we will adopt the value of those coefficients given by a $N=5$ fit.

IV. RESULTS

A. Single differential cross section

From Eq. (6) we see that β_0 is proportional to the SDCS and a test of the values found for β_0^E could be given by comparison with other authors. However, there are no experimental data available for the case of multicharged ions, so we look for a scaling relation between SDCS's for H^+ and those for the other projectiles. From experimental data on SDCS's obtained from different laboratories and high-energy ionization theories, Rudd *et al.* [17] have proposed an empirical expression for the SDCS corresponding to electron emission in proton-atom collisions. We will use this equation for evaluation of the SDCS for H^+-He collisions, which will be scaled for comparison with the SDCS we have obtained for the highly charged ions. There are two main scaling laws usually employed in ionization theory. One derives from first-order perturbation theory, and we call it Born scaling (BS):

$$\frac{d\sigma}{dE}(E,Z)=Z^2\frac{d\sigma}{dE}(E,1)\ . \tag{8}$$

This scaling rule is supposed to be valid in the region $Z/V<1$. The other scaling relation we study reads

$$\frac{d\sigma}{dE}(E,Z)=Z\frac{d\sigma}{dE}(E/Z,1)\ . \tag{9}$$

It was first found, by Olson and Salop [20], to be satisfied by the classical-trajectory Monte Carlo method (CTMC) and derived later by Janev and Preshnyakov [21], using the dipolar approximation and the atomic-orbital close-coupling method, for evaluation of the ionization total cross sections. We will refer to Eq. (9) as the Janev and Preshnyakov scaling (JPS). Recently, Rodri-

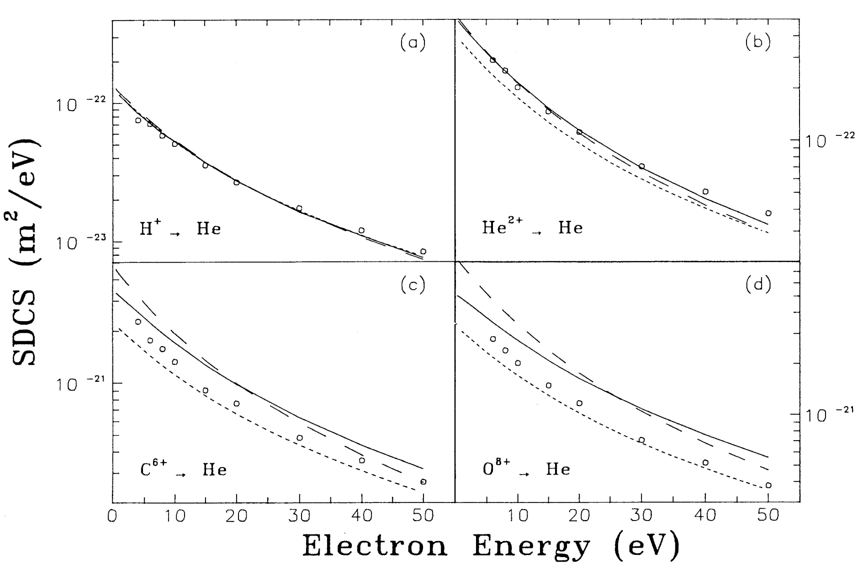

FIG. 1. SDCS for ionization at 1-MeV/amu impact energy: circles, experimental data; solid lines, CDW-EIS theory; long-dashed lines, BS of Rudd formula; short-dashed lines, JPS of Rudd expression.

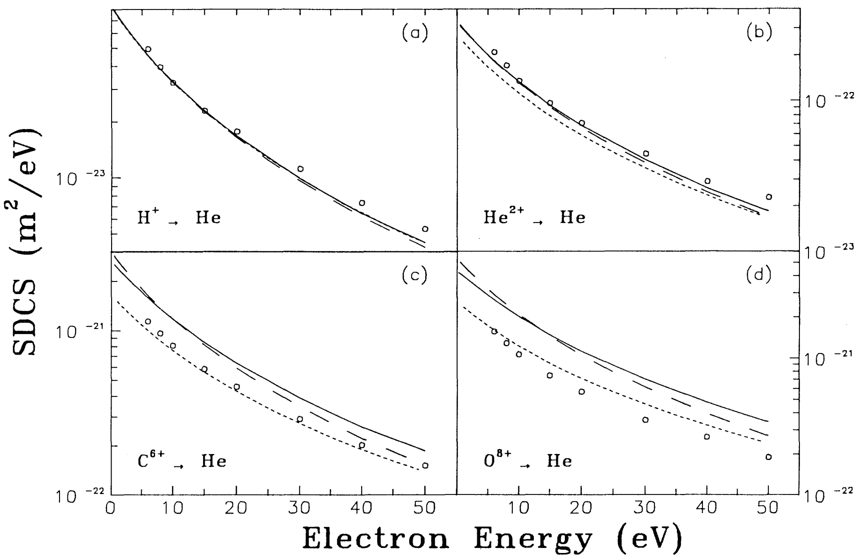

FIG. 2. As in Fig. 1 for 1.84-MeV/amu impact energy.

guez and Falcon [22] have determined that Eq. (9) is satisfied when the SDCS is calculated both in CTMC and CDW-EIS theories for hydrogen ionization in the region mediate energy.

From Figs. 1(a) and 2(a) we see the excellent agreement between Rudd's equation and the values for the SDCS obtained here for H^+ projectiles. For He^{2+} we have $Z/V \simeq 0.30$, and we are in the perturbative validity range where the Born scaling is appropriate, as can be observed in Figs. 1(b) and 2(b). However, as expected, saturation effects are evident as Z increases, and the SDCS grows more slowly than the Z^2 law. In Figs. 1(c), 1(d), 2(c), and 2(d) we compare JPS's and BS's of Rudd's equation for C^{6+} and O^{8+} projectiles with the SDCS obtained from the present fitting of experimental data. We observe that in general the JPS provides a better description than the BS, which is closer to theoretical values for the SDCS provided by CDW-EIS calculations.

B. Asymmetry parameters

In Figs. 3 and 4 we show the $\alpha_l^E(v)$ obtained by fitting the experimental data, and compare them with those resulting from Born and CDW-EIS approximations. The α_l^B given by the FBA should not depend on projectile charge, as the Z^2 dependence of the DDCS is contained in β_0^B. As expected, asymmetry parameters become smaller for increasing incident energy. From the selection rules mentioned before, α_1^B and $\alpha_{l>2}^B$ converge to zero as $v \rightarrow 0$, regardless of the incident energy. For small v, α_1^B and α_3^B have similar magnitude and opposite sign, therefore their joint contribution to the SEP asymmetry in the forward-backward direction is small. Meanwhile, α_2^B has a negative value, which increases with the incident energy, and has its physical origin in the contribution of the binary collisions to the electronic emission. Regarding the value of the experimental pa-

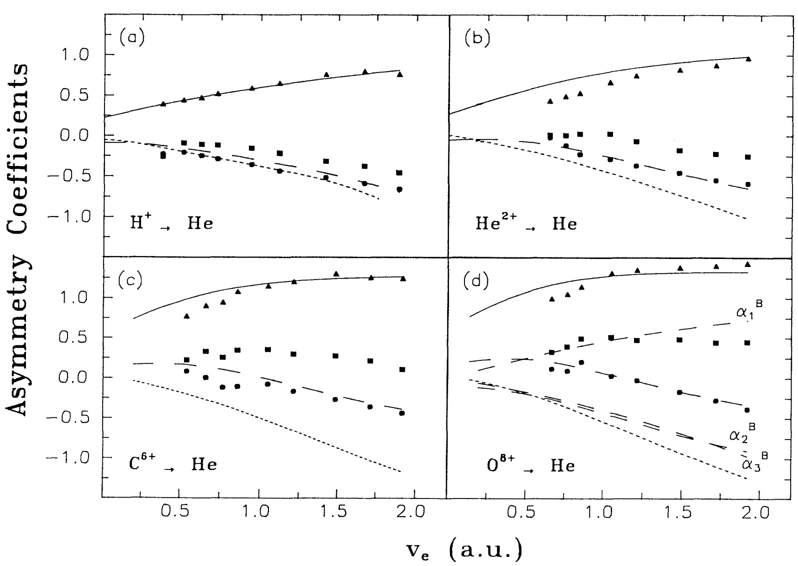

FIG. 3. Asymmetry parameters for 1-MeV/amu: α_1^E, triangles; α_2^E, squares; α_3^E, circles; α_1^C, solid lines; α_2^C, dashed-dotted lines; and α_3^C, short-dashed lines. Asymmetry parameters calculated in the FBA (long-dashed line) are the same for different projectiles, so they are shown only for oxygen.

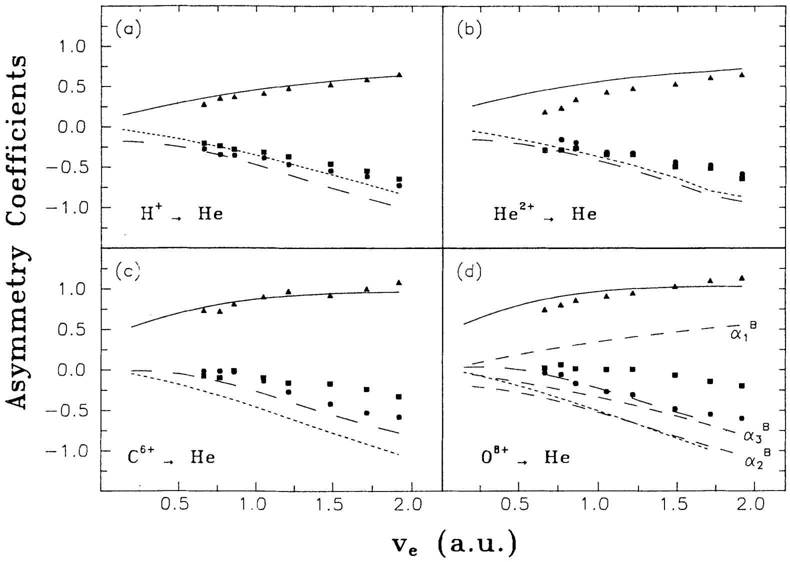

FIG. 4. As in Fig. 3 for 1.84-MeV/amu impact energy.

rameters, we note that α_1^E for H^+ and He^{2+} projectiles have the same value, indicating a perturbative behavior, within the experimental errors. The values of α_1^E increase with the projectile charge, but do not exhibit a scaling rule. For C^{6+} and O^{8+} ions they are of the same order, which is about twice the value for H^+, at low electron velocities. The α_1^C calculated using CDW-EIS theory show good agreement with the experimental values α_1^E for different projectiles and incident energies and do not vanish as v tends to 0. The limit value $\alpha_1^{E,C}$ ($v=0$) grows with Z, as should be expected, because this parameter below threshold is related to the dipole moment of the residual target system induced by the projectile [14].

In general, the values of α_2^E and α_3^E are smaller and show a flatter dependence on v than the theoretical ones, and agreement is poor, even taking into account the large numerical errors involved in the derivation of these experimental parameters. In the limit $v \to 0$, the α_2^C converges to a nonzero value, negative for H^+ and He^{2+} ions and positive for C^{6+} and O^{8+} projectiles, while α_3^C becomes zero in that limit. A similar behavior seems to be true for α_2^E and α_3^E, but we cannot be sure since a precise extrapolation is not possible in these cases. That change of sign in α_2 was also found, in theoretical calculations of the cross sections for excitation of H from $n=1$ to $n=2$ and 3 by nude projectiles, when the ratio V/Z decreases [6].

A compensation between the contribution of α_1^C and that of α_3^C to the DDCS is observed as v increases, and therefore the forward-backward asymmetry given by the CDW-EIS is smaller than that observed in the experimental data. This is to be expected, since it is known that this theory underestimates the DDCS in the two-center ridge region [19,23].

V. CONCLUSIONS

The main conclusion of this work is that the present analysis of existing experimental data on DDCS's for He-atom ionization confirms the existence of a strong asymmetry in the soft-electron emission induced by ion-atom collisions, and shows that post-collisional interaction between the projectile and the emitted electron is important in the SEP. This asymmetric emission is also predicted by the CDW-EIS theory, at least qualitatively.

The results are analyzed through the coefficients of a Legendre-polynomial expansion of the DDCS. The angle-independent factor β_0 in that expansion gives the energy SDCS, which is compared with the values resulting from scaling of the equation proposed by Rudd *et al.* [17], for H^+-He ionization. We propose two kinds of scaling, and we obtain that the JPS, defined by Eq. (9), gives a good description for the cases considered here. We find that the first asymmetry parameter α_1, which below threshold is associated with the target induced dipole, increases with Z and decreases with V, suggesting that it is generated by a post-collisional projectile-induced effect. The SDCS and α_1 satisfy Born scaling relations in the case of He^{2+}, as may be expected since in this case $Z/V<1$. However, as Z increases, deviations from the Z^2 law become important, but are smaller than those predicted by Eq. (9), indicating other possible scaling relations. In this direction, it would be desirable to have experimental data taken in the appropriate energy range to test different scaling laws. The coefficients obtained from experiments and from the CDW-EIS approach extrapolated to $v=0$ follow a Z dependence similar to that observed in those calculated below the ionization threshold in excitation of hydrogen atoms, as required by continuity. They have a smooth behavior for $v>0$ and can be approximated by a few terms of a power-series expansion in v. This points out that Eq. (2) gives an appropriate fitting scheme for the DDCS at low electron velocities.

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