Electron-impact-excitation cross sections of hydrogenlike ions

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Convergent close-coupling (CCC) and Coulomb-Born with exchange and normalization (CBE) methods are used to study electron-impact excitation of hydrogenlike ions. The $nl \rightarrow n'l'$ cross sections demonstrate (i) good agreement between the CCC and CBE results, (ii) a scaling over ion nuclear charge z, (iii) a domination of the dipole $(l'=l\pm 1)$ contributions in total $n \rightarrow n'$ cross sections, and (iv) significant effect of electron exchange in the energy range x < 3 (here x is the ratio of the incident electron kinetic energy ε to the transition energy $E_{n,n'}$). For ions with z>5 the $n \to n'$ cross sections obtained in the CCC and CBE approximations agree with each other to better than 10% for any x. An accuracy of the cross sections scaling over z^4 depends on z: for z=6-18 the scaling is accurate to better than 10% (quantitative analysis is done for n' < 7), for ions with z < 6 the cross sections deviate from the z^4 scaling more significantly (at x about unity). The $n \rightarrow n'$ cross sections are presented by a formula which fits our CCC and CBE results with an accuracy to better than 10% (for transitions with n < n' < 7 in ions with z > 5). The new Gaunt factor G(x) suggested for the widely used Van Regemorter formula [Astrophys. J. 136, 906 (1962)] makes this formula accurate to better than 50% in the x>3 range and to better than 20% in the x>100 range. It is shown that the semiempirical formula by Vainshtein, Sobelman, and Yukov [Electron-Impact Excitation Cross Sections of Atoms and Ions (Nauka, Moscow, 1973) provides an accuracy to better than 50% for any incident electron energy. For x < 2 this formula is accurate to better than 30%. These accuracy assessments are based on a comparison with our CCC and CBE results. [S1050-2947(97)00301-6]

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I. INTRODUCTION

Interpretation of spectroscopic measurements in plasma physics and astrophysics, simulation of kinetic and transport processes in nonequilibrium plasmas, radiative hydrodynamics, and some other fields of plasma physics require accurate cross sections for electron-impact-induced transitions in ions. In general, any inelastic cross section may be calculated by computer codes designed for this purpose (see, for example, Refs. [1-9]). Hundreds of cross sections are already calculated or determined experimentally for some intervals of incident electron energy. These results can be found in publications and in atomic data bases (see, for example, Ref. [9]). However, published cross sections are often insufficient for plasma physics and astrophysics, since data on many cross sections are missing or do not cover the entire energy range required for calculation of excitation rates, especially for non-Maxwellian plasmas.

In this paper, we present and discuss full-energy-range high-accuracy cross sections for electron-impact excitation of hydrogenlike ions. The paper is structured as follows. In Sec. II, we discuss briefly the $nl \rightarrow n'l'$ cross sections computed by the convergent close-coupling (CCC), close-

coupling (CC), and Coulomb-Born with exchange and normalization (CBE) methods. In Sec. III, we focus on the $n \rightarrow n'$ cross sections and the high-accuracy fitting formula for the cross sections with n < n' < 7 in ions with z > 5. In Secs. IV and V, the CCC and CBE results are used for improving the widely used semiempirical formulas and for assessing an accuracy of these formulas.

II. THE $nl \rightarrow n'l'$ CROSS SECTIONS

The CCC method is presented in Refs. [8,10]. The basic idea of the CCC approach to electron-ion collisions is to solve the coupled equations arising upon expansion of the total wave function in a truncated Laguerre basis of size N. This basis size is increased until convergence to a desired accuracy is observed. The usage of the Laguerre basis ensures that all states in the expansion are square integrable, and so gives a discretization of the target continuum as well as a good representation of the target true discrete spectrum. For sufficiently large N pseudoresonances, associated with the target continuum discretization, diminish substantially so that no averaging is necessary. The presented CCC calculations at all given energies are likely to be within 10% of the

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FIG. 1. Cross sections for transition $1s \rightarrow 2s$ in hydrogenlike ions with z=2-26.



true nonrelativistic model solution for the considered scattering systems. In general, the CCC cross sections are in excellent agreement with the experimental results available for various targets [8,10,11].

The CBE cross sections were calculated by the ATOM computer code [3]. In this code, the exchange is accounted for by the method of orthogonalized functions and the normalization is done by the K-matrix method using one own channel of the reaction [4].

Both CBE and CCC computer codes produce the cross sections for $nl \rightarrow n'l'$ transitions. These cross sections are denoted here by $\sigma_{z,nl,n'l'}(x)$ with

$$x = \varepsilon / E_{nn'}$$

being the ratio of the incident electron kinetic energy ε to the transition energy $E_{n,n'}$. The most important of the $nl \rightarrow n'l'$ cross sections, namely, the cross sections $\sigma_{z,1s,2s}(x)$ and $\sigma_{z,1s,2p}(x)$ are shown in Figs. 1 and 2 for a few ions with z from 2 to 26. The CC results are taken from Refs. [12–14]. Detailed quantitative analysis of the $nl \rightarrow n'l'$ cross sections will be published in a separate paper. The main conclusions of this analysis are as follows. (i) Scaling of the $nl \rightarrow n'l'$ cross sections over z^4 is very accurate for $x \ge 1$. For x about unity, the cross sections related to small z (i.e., to z = 2,3,4) deviate from the scaling significantly (see, for example, the cross sections for He⁺). In general, a deviation from the scaling depends on parameter p = (z-1)/z which is the ratio of a charge affecting an inci-



FIG. 2. Cross sections for transition $1s \rightarrow 2p$ in hydrogenlike ions with z=2-26.



FIG. 3. Cross sections for transition $1 \rightarrow 2$ in hydrogenlike ions with z=2-26.

Incident Electron Energy in Threshold Units x

dent electron (at a large distance from the target) to a charge affecting an optical electron [4]. Deviation of the cross sections from the z^4 scaling increases with deviation of p from unity, i.e., with the decrease of z. One can see this regularity in the cross sections presented in Figs. 1-3, where z changes from 2 to 26. (ii) Electron exchange is affecting the cross sections significantly in the energy range x < 3. This effect is increasing with the multipole order |l'-l|. (iii) Dipole $(l' = l \pm 1)$ contributions dominate over nondipole ones in the total $n \rightarrow n'$ cross sections. In particular, one can see that at $x \approx 1$ the $1s \rightarrow 2p$ cross section is larger than $1s \rightarrow 2s$ cross section by a factor of 4; with x the $1s \rightarrow 2p$ cross section goes down slower than $1s \rightarrow 2s$ one (namely, as $x^{-1}\ln x$ vs x^{-1}), therefore the total $1 \rightarrow 2$ cross section is almost exclusively due to the dipole channel. (iv) For z > 5the CCC, CC, and CBE cross sections usually agree with each other to better than 10%.

The last statement is correct for the energy values we considered, however, it may be wrong for narrow energy intervals in the vicinity of the excitation threshold (i.e., in certain intervals within the $x \approx 1$ domain) where the cross sections are contributed significantly by resonance excitation channels. Detailed analysis presented in Refs. [15–19] shows that the resonances may increase some cross sections up to an order of magnitude (within the energy intervals $\Delta x < 10^{-3}$). However, usually plasma physicists and astropysicists are not interested in such fine resolution of collisional cross sections. On the contrary, they operate with integrals over entire energy range, namely, with the excitation rates

$$R_{z,nl,n'l'}(\overline{\varepsilon},p) = \int_0^\infty \sigma_{z,nl,n'l'}(\varepsilon) v_e(\varepsilon) f_e(\varepsilon,\overline{\varepsilon},p) d\varepsilon,$$

therefore, the actual effect of the resonances on the collisional processes may be assessed by comparison of the rates calculated with an account for the resonances and without it. In the last formula, $v_e(\varepsilon)$ is the electron velocity,

 $f_e(\varepsilon,\overline{\varepsilon},p)$ is the electron energy distribution normalized by condition $\int_0^{\infty} f_e(\varepsilon,\overline{\varepsilon},p)d\varepsilon = 1$, $\overline{\varepsilon}$ is the average electron energy (in the case of the Maxwellian distribution, $\overline{\varepsilon}=3kT_e/2$), and p denotes all parameters of non-Maxwellian distributions. Calculations reported in Refs. [15–19] show that the resonances to dipole cross sections increase Maxwellian rates of these transitions by a few percent or less; rates of nondipole transitions increase more significantly but always less than +30%. Our estimates, based on the data of Refs. [15–19], show that contributions of resonances into total $n \rightarrow n'$ rates are less than +10% for any electron temperature reasonable for the existence of the hydrogenlike ion of interest.

III. TOTAL $n \rightarrow n'$ CROSS SECTIONS

The $n \rightarrow n'$ cross sections are denoted here by $\sigma_{z,n,n'}(x)$. They may be presented as sums over *l* and *l'*

$$\sigma_{z,n,n'}(x) = \sum_{l=0}^{n-1} g_{nl} g_n^{-1} \sum_{l'=0}^{n'-1} \sigma_{z,nl,n'l'}(x).$$
(1)

Here g_{nl} and $g_n = \sum_l g_{nl}$ are the statistical weights of states nl and n, respectively. Statistical averaging over l (which is reflected by the factor $g_{nl}g_n^{-1}$) is necessary because of the uncertainty of l in initial quantum states defined by quantum number n only. Summation over l' ensures the inclusion of all possible final states for a given n' of interest.

Figure 3 presents simple but important examples of the $n \rightarrow n'$ cross sections, namely, the cross sections $1 \rightarrow 2$ for ions with nuclear charges from 2 to 26. To emphasize the scaling of the cross sections over z^4 , we present scaled cross sections $z^4\sigma_{z,n,n'}(x)$.

In general, our analysis is based on three sets of results: (i) the CBE cross sections for all transitions with n < n' < 7in ions C⁵⁺, Ne⁹⁺, Al¹²⁺, Ar¹⁷⁺; (ii) the CCC cross sections for all transitions with n < n' < 5 in ions He⁺, C⁵⁺,

TABLE I. Coefficients $\alpha_{nn'}$, $\beta_{nn'}$, $\gamma_{nn'}$, $\delta_{nn'}$, and $\zeta_{nn'}$ for fitting function (2).

n	n'	$\alpha_{nn'}$	$\beta_{nn'}$	$\gamma_{nn'}$	$\delta_{nn'}$	$\zeta_{nn'}$
1	2	3.22	0.357	0.00157	1.59	0.764
1	3	0.452	0.723	0.0291	-0.380	0.834
1	4	0.128	-0.0300	0.163	-0.150	0.185
1	5	0.0588	-0.0195	0.0803	-0.0649	0.0776
1	6	0.0321	-0.0115	0.0458	-0.0374	0.0441
2	3	173	46.7	-94.5	358	-102
2	4	16.7	-8.32	12.6	22.5	-3.44
2	5	4.47	-5.54	8.10	3.52	0.820
2	6	1.94	-2.69	4.43	0.461	1.54
3	4	1880	204	-1280	4860	-1620
3	5	164	-236	128	458	-247
3	6	-2.71	-468	268	161	-304
4	5	4800	-55 100	18 100	41 400	-48 800
4	6	456	-4530	2230	2870	-3570
5	6	75 000	247 000	-172 000	84 700	123 000

Al¹²⁺; and (iii) the CC results available for transition $1 \rightarrow 2$ in ions C⁵⁺, O⁷⁺, Ar¹⁷⁺, Fe²⁵⁺ [12–14]. For $x \ge 1$ all scaled cross sections studied are independent of z to an accuracy better than 1%. However, for x about unity an accuracy of the scaling is smaller and depends on z: the scaling is accurate to within 5% for z=10-26, and to within 10% for z=6 (except for $5\rightarrow 6$ cross section in C⁵⁺ which deviates from the scaling law by 17% at $x\rightarrow 1$). For z<6 a deviation from the z^4 scaling is more significant, for example: 40% for transition $1\rightarrow 2$ in He⁺ and a factor of 3 for transition $5\rightarrow 6$ in He⁺. As was already mentioned, an accuracy of the scaling is determined by the ratio (z-1)/z.

To present quantitatively all $n \rightarrow n'$ cross sections computed by CCC and CBE methods, we fitted them using a simple analytical function. Taking account of the z^4 scaling and analysis presented in Ref. [20] the fitting function was chosen to be

$$\sigma_{z,n,n'}^{f}(x) = \pi a_{0}^{2} z^{-4} x^{-1} (\alpha_{n,n'} \ln x + \beta_{n,n'} x^{-1} \ln x + \gamma_{n,n'} + \delta_{n,n'} x^{-1} + \zeta_{n,n'} x^{-2}).$$
(2)

Here a_0 is the Bohr radius. The coefficients $\alpha_{n,n'}$, $\beta_{n,n'}$, $\gamma_{n,n'}$, $\delta_{n,n'}$, and $\zeta_{n,n'}$ are listed in Table I. For energy interval $1 \le x \le 100$, the fit is accurate to better than 10% for all of the cross sections studied (z=6-26) except for C⁵⁺ the 5 \rightarrow 6 cross section. For this one, the inaccuracy increases to 17% at $x \rightarrow 1$.

Coefficients $\alpha_{n,n'}$, $\beta_{n,n'}$, $\gamma_{n,n'}$, $\delta_{n,n'}$, $\zeta_{n,n'}$ provide an accurate fit of the CCC and CBE results in the interval $1 \le x \le 100$ but they do not provide correct asymptotic behavior of the cross sections for x > 100. The calculations show that for $x \ge 10$ the CCC and CBE cross sections decrease with x as $x^{-1}\ln x$ (this asymptotic is caused by a dipole channel), therefore, for x > 100 the cross sections may be calculated using an expression

$$\sigma_{z,n,n'}(x > 100) = \sigma_{z,n,n'}(100) \frac{x^{-1} \ln x}{100^{-1} \ln 100}$$

$$\approx 21.7\sigma_{z,n,n'}(100)x^{-1}\ln x.$$
 (3)

An accuracy of this expression equals to an accuracy of the cross section at x = 100, i.e., is to within 10%.

IV. THE VAN REGEMORTER FORMULA

Expressions (2) and (3) may be used in applications which require high-accuracy cross sections. For estimates, it is desirable to have a simpler expression which does not use a table of coefficients. Frequently, such estimates are based on the Van Regemorter formula [4,5,21–26]. For $n \rightarrow n'$ transitions this formula may be presented as follows:

$$\sigma_{z,n,n'}^{VR}(x) = \pi a_0^2 \frac{8 \pi f_{nn'}}{\sqrt{3}} \frac{\mathcal{R}^2}{E_{nn'}^2} \frac{G(x)}{x}.$$
 (4)

Here $f_{nn'}$ is the absorption oscillator strength, $\mathcal{R} = 13.6 \text{ eV}$ is the Rydberg energy unit, and G(x) is the effective Gaunt factor which may be treated as a fitting function of order unity.

To find an accurate expression for the *n*-independent function G(x), we first use the fitting function (2) and Eq. (4) to introduce the Gaunt factor $G_{nn'}(x)$ for each of the transitions studied

$$G_{nn'}(x) = x \sigma_{z,n,n'}^f(x) \left(\pi a_0^2 \frac{8 \pi f_{nn'}}{\sqrt{3}} \frac{\mathcal{R}^2}{E_{nn'}^2} \right)^{-1}.$$

The Gaunt factors for all transitions with n < n' < 7 are shown by dotted curves in Fig. 4. The curves are not labeled because they are shown only in order to demonstrate the small spread of functions $G_{nn'}(x)$ near their mean function

$$G(x) = 0.349 \ln x + 0.0988 + 0.455x^{-1},$$
 (5)

which is shown by a bold solid curve. We recommend function (5) as an effective Gaunt factor for the Van Regemorter formula (4).

Bold dotted-dashed curves in Fig. 4 show a $\pm 50\%$ corridor around this G(x). One can see that for $x \approx 1$ some dotted curves deviate from G(x) by more than a factor of 2, but for x > 5 the spread of the dotted curves is smaller (namely, to within $\pm 50\%$), and for x = 100-1000 the spread is to within 20%.

V. THE VSY FORMULA

The Van Regemorter formula (4) is most accurate for $x \ge 1$. Therefore, this formula fits applications which require an accurate account of suprathermal electrons (e.g., pulsed-power devices, subpicosecond lasers, solar flares). However, there are non-Maxwellian plasmas with an overpopulated low-energy part of the electron distribution function, e.g., plasmas produced by high-power microwave devices or by lasers with nonrelativistic intensity of radiation (for our example, it is enough to have a free-electron oscillation energy less than the mean energy of the chaotic motion of the electron). Estimates of kinetic coefficients for such plasmas, require cross sections accurate in the low-energy range (x=1-10). A semiempirical formula suitable for this case

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FIG. 4. Gaunt factor G(x) for the Van Regemorter formula (4). Dotted curves demonstrate functions $G_{nn'}(x)$.

was suggested by Vainshtein, Sobelman, and Yukov (VSY) [21,4]. We rewrite this formula as follows:

$$\sigma_{z,n,n'}^{VSY}(x) = \frac{\pi a_0^2}{\sqrt{n'}} \left(\frac{\mathcal{R}}{I_n - I_{n'}}\right)^2 \left(\frac{I_{n'}}{I_n}\right)^{3/2} \frac{F(x)}{x}, \quad (6)$$

where I_n is the optical electron binding energy and

$$F(x) = 14.5 \ln x + 4.15 + 9.15x^{-1} + 11.9x^{-2} - 5.16x^{-3}$$
(7)

is the fitting function which provides a good fit to the CCC, CC, and CBE cross sections discussed above. Being interested in an easy-to-use formula, we looked for a function F(x) which is independent in z, n, and n', although initially



[21,4] trial functions F(x) were fitted to each of the transitions studied. Using the expression $I_n = \mathcal{R}z^2n^{-2}$ for the binding energy, formula (6) may be presented as follows:

$$\sigma_{z,n,n'}^{VSY}(x) = \frac{\pi a_0^2}{z^4} n^7 \sqrt{n'} [(n')^2 - n^2]^{-2} \frac{F(x)}{x}.$$
 (8)

Function (7) is shown by the bold solid curve in Fig. 5. Dotted curves demonstrate functions $F_{nn'}(x)$ obtained by replacing $\sigma_{z,n,n'}^{VSY}(x)$ in expression (8) by function (2)

$$F_{nn'}(x) = \frac{z^4 x \sigma_{z,n,n'}^f(x)}{\pi a_0^2} \frac{[(n')^2 - n^2]^2}{n^7 \sqrt{n'}}.$$

FIG. 5. Function F(x) for the VSY formula (8). Dotted curves demonstrate functions $F_{nn'}(x)$.

These dotted curves are not labeled because they are shown only in order to demonstrate their small deviation from the function F(x). The bold dashed curves show a $\pm 30\%$ corridor around F(x) while the bold dotted-dashed curves show a $\pm 50\%$ corridor. One can see that for x < 2 the VSY formula is accurate to within 30%. For x=1-10 this formula is accurate to within 50%. For larger electron energy (x > 10), estimates of the cross sections are more accurate if based on the Van Regemorter formula (4).

VI. CONCLUSIONS

The cross sections for electron-impact-induced transitions in He⁺, C⁵⁺, Ne⁹⁺, Al¹²⁺, and Ar¹⁷⁺ are calculated using the CCC and CBE methods (for transitions with n < n' < 7).

The $nl \rightarrow n'l'$ cross sections demonstrate (i) good agreement between the CCC and CBE results, (ii) a scaling over z^4 , which is very accurate for $z \ge 1$ and $x \ge 1$, (iii) significant effect of electron exchange in the energy range x < 3, and (iv) a domination of the dipole contributions in total $n \rightarrow n'$ cross sections.

The $n \rightarrow n'$ cross sections demonstrate an agreement to better than 10% between the CCC and CBE results for z > 5.

A scaling of the $n \rightarrow n'$ cross sections over z^4 is accurate

to within a few percent for ions with large nuclear charge $(z \ge 1)$. For ions with z about unity, a deviation from the scaling is significant (at x about unity). For $x \ge 1$ the z^4 scaling is accurate for all ions and transitions. For each z, an accuracy of the scaling is higher for larger transition energy. Quantitative results are presented by formula (2) which fits our CCC and CBE cross sections with an accuracy to better than 10%.

Semiempirical formulas (4) and (8) together provide an accuracy to within 50% for any energy: for x < 2 the VSY formula (8) is accurate to within 30%; for 2 < x < 10 this formula is accurate to within 50%; for x > 10 an accuracy to better than 50% is provided by the Van Regemorter formula (4).

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