K-shell ionization of atoms by electron and positron impact

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In the plane-wave Born approximation (PWBA), scaling relations for K-shell generalized oscillator strengths and energy-loss cross sections of atoms are given. The total K-shell ionization cross sections, obtained at high impact energy, are used to obtain the Bethe collisional parameter c_K for atoms ranging from carbon to gold. These values of c_K are, in general, significantly different from those obtained previously with the help of Fano plots at relatively low impact energies. Furthermore, using Hippler's modification of the PWBA [Phys. Lett. A **144**, 81 (1990)], total K-shell ionization cross sections of various atoms by electron and positron impact are calculated over a wide energy range. The electron-impact ionization cross sections for light atoms are in satisfactory agreement with the experimental data.

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The K-shell ionization cross sections of atoms find their applications in a number of fields. For example, they are needed in various types of material characterization such as electron-probe microanalysis, Auger-electron spectroscopy, electron energy-loss spectroscopy [1], etc. They are also required in the modeling of the interactions of ionizing radiation with matter. Hence a number of attempts have been made to obtain K-shell ionization cross sections, Q^-, by *electron* impact for different atoms over a wide energy range. The developments in this field up to the early 1980's have been reviewed by Powell [1]. However, investigations of *positron*-impact ionization of atoms have started only recently. Only a few experimental investigations [2–8] have been carried out to measure the total (sum over all atomic shells) positron-impact ionization cross sections. So far, no experimental measurement of Q^+, the K-shell ionization cross sections by positron impact for any atom having more than two electrons, has been carried out. Only the cross-section ratios Q^-/Q^+ for silver [9] and copper [9–11] have been measured. These measurements show that at low impact energies the ratio Q^-/Q^+ is greater than unity. This observation cannot be explained by the first Born approximation calculations in which the cross sections are the same for positron and electron impacts. Nevertheless, it is of interest to examine the existence of scaling relation(s) in the plane-wave Born approximation (PWBA) similar to that recently pointed out by Mayol and Salvat [12] and by Khare, Saksena, and Ojha [13] for K-shell photoionization cross sections (optical oscillator strengths) of atoms in the hydrogenic approximation. Furthermore, evaluation of the Bethe collisional parameter c_K from electron-impact ionization cross sections for atoms, just like evaluation of Bethe size parameter b_K by Khare, Saksena, and Ojha [13] from photoionization cross sections, is also of interest.

It is known that the inclusion of exchange effects (for example, with the help of Ochkur approximation) in PWBA reduces [14] Q^-, thus yielding $Q^-/Q^+<1$, which is contrary to the experimental observations. Recently, Hippler [15] has introduced a simple correction to PWBA which takes into account the acceleration of the incident electron and deceleration of the incident positron by the atomic nuclear field. His calculated K-shell ionization cross sections of argon atom by electron impact are in very good agreement with the experimental data of Hippler *et al.* [16] and of Tawara *et al.* [17] even for energies close to threshold energy. He has also calculated the ratio Q^-/Q^+ for the silver atom and got good agreement with the experimental data for silver and copper atoms [9–11]. To explore the extent of the applicability of Hippler's method we have, in the present investigations, calculated $Q^\pm$ for a number of atoms over an extended energy range and have compared them with the available experimental data.

In the plane-wave Born approximation the double-differential cross section for the ionization of complex atoms by positrons or electrons of energy E is given by [18]

$$dQ(E,W,K^2)=\frac{4\pi}{E}\frac{1}{W}\frac{\partial f(W,K^2)}{\partial W}d(\ln K^2)dW\ , \quad (1)$$

where $\partial f(W,K^2)/\partial W$ is the generalized oscillator strength per unit energy range, for the ionizing collision in which the projectile loses an energy equal to W and its momentum changes by K. We express energy in the units of Rydberg and length in the units of first Bohr radius, unless specified otherwise. The double-differential ioniza-

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tion cross section is evaluated in the hydrogenic approximation [18]. It is well known that due to external screening the experimental K-shell ionization potential I_K is less than the hydrogenic K-shell ionization potential I_s. Hence the ratio $p=I_K/I_s$ is less than unity for all atoms except for the hydrogen atom for which $p=1$.

Now we introduce new variables α^2 and β^2 as

$$\beta^2=\frac{K^2}{I_s}\ , \quad \alpha^2=\frac{W-I_s}{I_s}\ , \tag{2}$$

and obtain from (1), in the hydrogenic approximation,

$$\frac{\partial f(W,K^2)}{\partial W}=\frac{1}{I_s}\frac{\partial f(\alpha^2,\beta^2)}{\partial \alpha^2}\ , \tag{3a}$$

where

$$\frac{\partial f(\alpha^2,\beta^2)}{\partial\alpha^2}=\frac{2^8(1+\alpha^2)\{\beta^2+1/3(1+\alpha^2)\}}{\{1+2(\beta^2+\alpha^2)+(\beta^2-\alpha^2)^2\}^3}F(\beta^2,\alpha)\ , \tag{3b}$$

with

$$F(\beta^2,\alpha)=\exp\left\{-\frac{2}{\alpha}\arctan\left[\frac{2\alpha}{\beta^2+1-\alpha^2}\right]\right\} \times\{1-\exp(-2\pi/\alpha)\}^{-1}\ ,\alpha^2\geq 0\ , \tag{4a}$$

and

$$F(\beta^2,\alpha)=\exp\left\{\frac{-1}{(-\alpha^2)^{1/2}} \times\ln\left[\frac{\beta^2+[1+(-\alpha^2)^{1/2}]^2}{\beta^2+[1-(-\alpha^2)^{1/2}]^2}\right]\right\}\ ,\ \alpha^2<0\ . \tag{4b}$$

It is evident from Eq. (3) that the generalized oscillator strength $\partial f(W,K^2)/\partial W$ is different for different atoms. However, the scaled oscillator strength $\partial f(\alpha^2,\beta^2)/\partial\alpha^2$ is the same function of α^2 and β^2 for all atoms. Hence $\partial f(\alpha^2,\beta^2)/\partial\alpha^2$ generates a universal Bethe surface when plotted as a function of α^2 and β^2. It is easy to see that Eqs. (3) and (4) reduce to Eq. (16) of Mayol and Salvat [12] and to Eqs. (1) and (2), respectively, of Khare, Saksena, and Ojha [13] for $\beta^2=0$. Thus the present scaling relation for the generalized oscillator strength is a natural extension of the scaling relation for the optical oscillator strength.

Now the integration of Eq. (1) over K^2 yields the energy-loss cross section per unit energy range. In terms of the variables β^2 and α^2 we obtain

$$dQ(U,\alpha^2)=\frac{1}{I_s^2}\frac{4\pi}{U}\frac{d\alpha^2}{(1+\alpha^2)}\int_{\ln\beta^2_{\rm min}}^{\ln\beta^2_{\rm max}}\frac{\partial f(\alpha^2,\beta^2)}{\partial\alpha^2}d(\ln\beta^2)\ , \tag{5}$$

where U is the hydrogenic overvoltage E/I_s and

$$\beta^2_{\rm max,\,min}=2U-1-\alpha^2\pm 2[U(U-1-\alpha^2)]^{1/2}\ . \tag{6}$$

We again notice that $I_s^2dQ(U,\alpha^2)$ is the same function of U and α^2 for all atoms and we thus obtain a second scaling relation. If U was defined as equal to E/I_K, then such a scaling relationship would not have existed.

To evaluate the total K-shell ionization cross section $Q^{\pm}(U)$ in the plane-wave Born approximation, Eq. (5) is integrated over α^2. If the projectiles are electrons, the possibility of exchange scattering should be included in the expression for $Q^{-}(U)$. Furthermore, as remarked earlier, another important effect which should be included in the theory for the calculation of $Q^{\pm}(U)$ is the distortion of the plane waves by the atomic field. A simple way to include such effects within the framework of the plane-wave Born approximation has been proposed recently by Hippler [15]. His method has given encouraging results. Hence, in the present investigation, we have adopted identically the same method to obtain $Q^{\pm}(U)$ for a number of atoms ranging from carbon to gold and U varying from 1 to 100. These cross sections are referred to as Coulomb-corrected cross sections. The values of I_K are taken from the table of Veigele [19] and $I_s=(Z-s)^2$, where Z is the atomic number of the target. Following Slater [20] the value of the inner screening constant is taken as 0.3.

For high values of U the total cross section, according to the Bethe theory, is given by [1]

$$I_K^2Q^{\pm}(U)=\frac{4\pi}{U}pZ_Kb_K\ln(c_KU)\ , \tag{7}$$

where Z_K is the number of electrons in the K shell. The Bethe size parameter b_K can easily be calculated by taking optical oscillator strength $\partial f(\alpha^2,0)/\partial\alpha^2$ as input and evaluating the following integral:

$$Z_Kb_K=p\int_{p-1}^{\infty}\frac{d\alpha^2}{(1+\alpha^2)}\frac{\partial f(\alpha^2,0)}{\partial\alpha^2}\ . \tag{8}$$

To evaluate the Bethe collisional parameter c_K, the generalized oscillator strengths are to be integrated [21]. However, in the present investigation, we have employed the Born values of $Q^{\pm}(U)$ at $U=400$ and Z_Kb_K from Eq. (8) to determine c_K from Eq. (7). As expected, at $U=400$ there is practically no difference between Born and Coulomb corrected cross sections. Table I shows that at $U=400$ the value of c_K for the hydrogen atom has reached its asymptotic value (=83) given by Bethe [18]. Hence we expect that the present values of c_K for other

TABLE I. The values of p and Bethe parameters b_K and c_K for K-shell ionization of atoms in the plane-wave Born approximation.

Atom	p	b_K	c_K
C	0.644	0.600	6.57
N	0.659	0.577	7.21
O	0.660	0.575	7.30
Ne	0.678	0.551	8.13
Al	0.711	0.509	10.1
Ar	0.751	0.463	13.1
Ni	0.798	0.418	18.1
Ag	0.860	0.369	28.1
Au	0.958	0.306	59.3
H	1.000	0.283	83.0

TABLE II. Scaled Coulomb-corrected K-shell ionization cross sections $I_K^2 Q^-(U)$ (in 10^{-14} cm^2 eV^2) of atoms by *electron* impact.

U \ Atom	C	N	O	Ne	Al	Ar	Ni	Ag	Au
1.00	2.76	2.67	2.66	2.57	2.37	2.11	1.78	1.30	0.424
1.40	3.54	3.51	3.50	3.46	3.37	3.26	3.11	2.90	2.51
2.00	3.75	3.74	3.73	3.72	3.69	3.64	3.59	3.51	3.35
3.00	3.51	3.51	3.51	3.51	3.51	3.51	3.50	3.49	3.45
4.00	3.17	3.18	3.18	3.18	3.19	3.20	3.21	3.22	3.23
5.00	2.87	2.87	2.87	2.88	2.89	2.91	2.92	2.94	2.96
7.00	2.39	2.39	2.40	2.40	2.41	2.43	2.45	2.47	2.51
10.00	1.91	1.92	1.92	1.92	1.93	1.95	1.96	1.98	2.02
20.00	1.17	1.17	1.17	1.18	1.18	1.19	1.19	1.21	1.23
30.00	0.859	0.860	0.860	0.860	0.863	0.867	0.872	0.879	0.893
40.00	0.685	0.685	0.685	0.686	0.687	0.689	0.692	0.697	0.706
50.00	0.572	0.572	0.572	0.573	0.573	0.574	0.576	0.580	0.587
70.00	0.434	0.434	0.434	0.434	0.434	0.434	0.435	0.437	0.441
100.00	0.324	0.323	0.323	0.323	0.322	0.322	0.322	0.323	0.325

atoms are also sufficiently accurate. Furthermore, just like b_K, the values of c_K also vary over a substantial range, from 6.57 for carbon to 83.0 for hydrogen. These values of c_K are quite different from those obtained by other investigators using Fano plot (see Table I of Powell [22] and also Table 6.2 of Powell [1]).

Let us now consider electron-impact ionization. The present values of $I_K^2 Q^-(U)$ are shown in Table II. The table shows that the cross section attains its maximum value at about $U=2$ for all atoms except gold for which the maximum in cross section occurs at about $U=3$. We also notice that at low U the value of $I_K^2 Q^-(U)$ decreases with the increase of p but beyond the maxima ($U \sim 3$) the trend is reversed. Nevertheless, the variation in the values of $I_K^2 Q^-(U)$ as one moves from carbon to gold is observed to be not more than 5% for $U \geq 3$. Such a scaling procedure is also supported by the experimental data [1,22].

In Figs. 1 and 2 we have compared Coulomb-corrected cross sections (curve A) and the Bethe cross sections (curve B) with the experimental data for carbon, a light atom, and silver, a relatively heavy atom. The Bethe cross sections are obtained from Eq. (7) with p, b_K, and c_K taken from Table I. It may be noted that Khare and Prakash [23] have also calculated the Bethe cross sections but they took empirically $b_K=0.57$ and $c_K=2.42$, which in view of the present calculations (see Table I) may not be regarded as quite appropriate. For the sake of clarity of figures only the recent experimental data, tabulated by Long *et al.* [24], are shown. In Fig. 1 the present cross sections (curve A) for carbon are compared with two sets of experimental data obtained by Tawara, Harrison, and deHeer [17] and by Hink and Paschke [25]. Bethe cross sections are also shown in the figure by curve B. As expected, curve A lies below curve B and approaches it

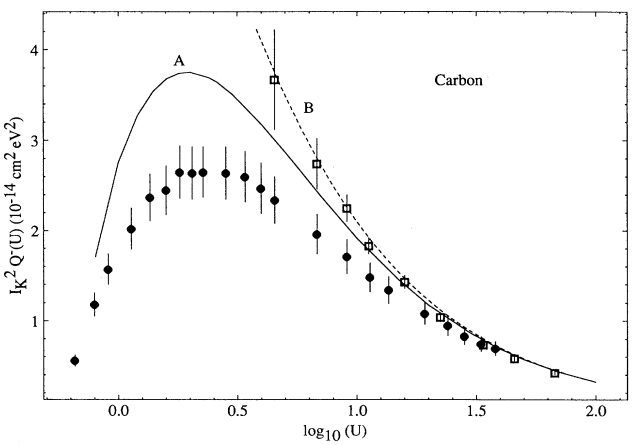

FIG. 1. Variation of $I_K^2 Q^-(U)$ with hydrogenic overvoltage U for the K-shell ionization of carbon atom by electron impact. Curves A and B show the present Coulomb-corrected and the Bethe cross sections, respectively. Solid circles and open squares represent the experimental cross sections of Tawara *et al.* [17,24] and of Hink *et al.* [24,25], respectively.

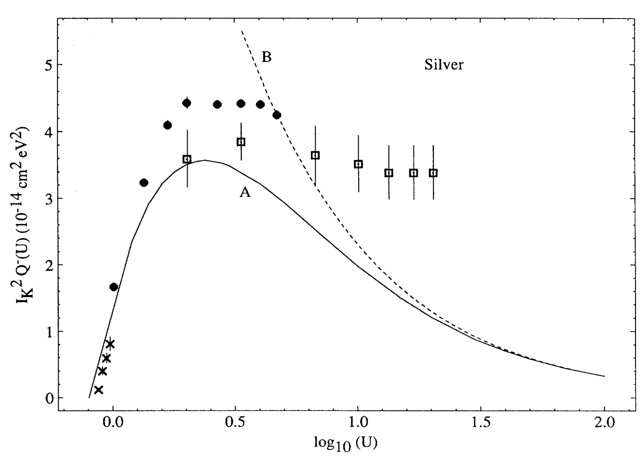

FIG. 2. Same as Fig. 1 except that the atom is silver. Open squares, crosses, and solid circles represent the experimental cross sections of Kiss *et al.* [24,26], Shima *et al.* [24,27], and Davis *et al.* [24,28], respectively.

TABLE III. Scaled Coulomb-corrected K-shell ionization cross setions $I_K^2 Q^+(U)$ (in 10^{-14} cm^2 eV^2) for atoms by *positron* impact.

U \ Atom	C	N	O	Ne	Al	Ar	Ni	Ag	Au
1.00	0.135	0.116	0.113	0.094	0.064	0.038	0.018	0.005	
1.40	0.779	0.724	0.718	0.659	0.555	0.443	0.336	0.226	0.109
2.00	1.94	1.88	1.87	1.81	1.70	1.52	1.35	1.13	0.829
3.00	2.83	2.81	2.81	2.78	2.73	2.66	2.57	2.44	2.20
4.00	2.93	2.93	2.93	2.92	2.92	2.91	2.89	2.85	2.77
5.00	2.78	2.79	2.79	2.80	2.81	2.83	2.84	2.85	2.85
7.00	2.40	2.41	2.42	2.43	2.45	2.47	2.50	2.54	2.59
10.00	1.95	1.95	1.96	1.96	1.98	2.01	2.03	2.07	2.13
20.00	1.19	1.19	1.19	1.20	1.21	1.22	1.23	1.25	1.28
30.00	0.871	0.872	0.872	0.874	0.879	0.884	0.892	0.903	0.923
40.00	0.692	0.693	0.693	0.694	0.696	0.700	0.705	0.712	0.726
50.00	0.578	0.578	0.578	0.579	0.580	0.582	0.585	0.590	0.600
70.00	0.438	0.437	0.437	0.437	0.438	0.439	0.441	0.443	0.449
100.00	0.325	0.325	0.325	0.325	0.324	0.324	0.325	0.326	0.329

asymptotically. The figure shows a good qualitative agreement between the curve A and the experimental data. The position of the maximum of the cross section $Q^-(U)$ is also well reproduced by the theory. However, the curve A lies between the two experimental sets of data over most of the energy range. Considering the differences among various experimental cross-section values, the agreement between the theoretical curve A and the experiment may be regarded as satisfactory over the entire range of U. Similar agreements have been obtained for neon, argon, and nickel atoms. However, for silver atom, Fig. 2 shows that for intermediate and large values of U the theory underestimates the cross sections. At the larger values of U a rather big difference between the theoretical and the experimental cross sections [26–28] is noticed. Similar disagreement between the theory and the experiment is found for gold atom as well.

Let us now consider cross sections for positron-impact ionization. Table III shows our Coulomb-corrected cross sections. As expected, at low values of U, these cross sections are smaller than those for electron impact. The difference between the two decreases with the increase of U. At about $U=6$, the cross section curves for positron and for electron impacts cross and, eventually, merge at large values of U. Furthermore, for positron impact the value of $U(\sim 4)$ at which the cross section has a maximum is higher than that for the electron case. Just like the case of electron impact, for $U \geq 5$ the values of $I_K^2 Q^+(U)$ increase with p whereas for $U<5$ it is just the opposite. As remarked previously, no experimental values of the cross sections for the K-shell ionization by positron impact are available for any atom having more than two electrons.

Another way to compare the theory with the experiments is through the ratio $Q^-(U)/Q^+(U)$ which has been measured for silver and copper [9–11]. Hippler [15] calculated this ratio for silver and compared it with the experimental data of Ebel *et al.* [9], Ito *et al.* [10], and Schultz and Campbell [11]. However, due to an oversight, the theoretical curve shown in Fig. 2 of his paper [15] is in error [29]. The corrected curve, generated in the present investigations, is shown in Fig. 3 along with the experimental ratios Q^-/Q^+ for silver and copper. A good agreement between the theory and the experiment is evident.

Finally, we conclude that the plane-wave approximation yields scaling relations for the generalized oscillator strengths and the energy-loss cross sections similar to the one noticed by Mayol and Salvat [12] and by Khare, Saksena, and Ojha [13] for the optical oscillator strengths in the hydrogenic approximation. The calculation shows that at high impact energies ($U \geq 10$) the scaled ionization cross sections $I_K^2 Q^{\pm}(U)$ are also nearly independent of the target atom. Using Born cross sections we have also obtained new values of the Bethe collisional parame-

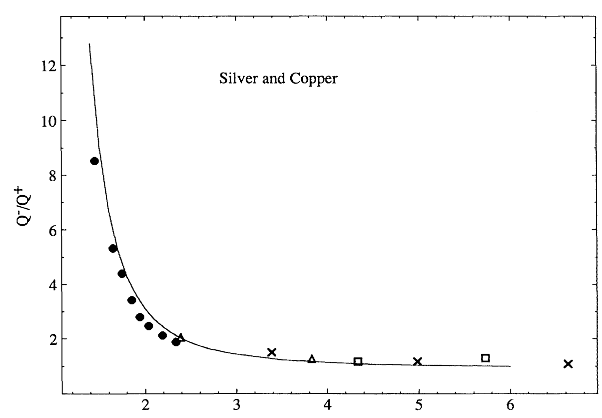

FIG. 3. Variation of the ratio $Q^-(U)/Q^+(U)$ with U. The solid curve shows the present results for silver atom. Solid circles represent the experimental data of Ebel *et al.* [9] for silver. Open squares, crosses, and open triangles represent the experimental cross-section ratios for copper obtained by Ebel *et al.* [9], Ito *et al.* [10], and Schultz and Campbell [11], respectively.

ter c_K for a number of atoms. Furthermore, a simple correction to PWBA, as proposed by Hippler [15], to take into account the acceleration of the incident electron gives K-shell ionization cross sections for light atoms which are in satisfactory agreement with the experimental data. However, for the heavier atoms this method underestimates the cross sections at intermediate and high values of U. The underestimation is found to be large even at those energies where the Coulomb corrections and the exchange effects are small and the Coulomb-corrected cross sections, using Hippler's method, are almost the same as the Born cross sections. Such a breakdown of the method for heavier atoms has also been noticed for the scaled photoionization cross sections [13] and it indicates that the theory should include the relativistic effects. The method, however, provides good values of the ratio $Q^-(U)/Q^+(U)$ even for heavier atoms.

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