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Electron capture from K shells by fully stripped ions

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Cross sections for electron capture from inner shells by fully stripped ions are calculated and compared with data for K-shell vacancy production. A procedure for inclusion of the relativistic effect is developed, and the scheme of calculations is illustrated through sample evaluations of electron-capture cross sections.

I. INTRODUCTION

We have developed formulas for electron capture from inner shells by fully stripped ions and have shown that reliable cross sections can be obtained[1,2] *without* semiempirical scaling factors.[3] Such factors are still being endorsed, for example, in recent publications of Gray and his co-workers.[4] Our approach goes beyond the first Born approximation with the neglected internuclear interaction in the perturbing potential, i.e., the Oppenheimer-Brinkman-Kramers (OBK) approximation,[5] and yet it does not require involved numerical procedures.[6] Although cast in terms of the formulas derived in an OBK approach, this analysis should not be viewed as merely its modification. For ions of low velocity in comparison with the orbital velocity of innershell electrons, the effects of Coulomb deflection and increased electron binding were accounted for[1] in a manner similar to that of Brandt and his co-workers[7] in the theory for direct ionization to the continuum of the target atom. Our low-velocity results were joined, through an expedient interpolation formula, with the high-velocity predictions obtained in the second Born approximation.[1] In this approximation, Drisko's formula[8] for the electron transfer from hydrogen ($Z_2=1$) to proton ($Z_1=1$) was generalized[1,9] for electron capture in the target-projectile collision systems with arbitrary atomic numbers Z_2 and Z_1.

Our original electron-capture formulas[1] have been modified[2] so that, to be consistent with the treatment of this effect in the direct ionization theory,[10,11] the binding effect was reduced. In Sec. II, we summarize the calculations and introduce the method which—in an analogous manner to the procedure developed recently for direct inner-shell ionizations[11]—reproduces the cross sections based on a relativistic description of the target atom. A detailed comparison of K-shell ionization cross sections with theoretical predictions is presented in Sec. III. Section IV contains a summary of this work. In the Appendix, sample calculations of electron-capture cross sections are delineated. They should provide a recipe for the use of the present approach. The scheme of calculations presented in the Appendix can also be easily followed and applied to the evaluation of the electron capture from the L subshells.[12] Except in the figures and the Appendix, atomic units are used throughout.

II. ANALYTICAL CALCULATIONS

Cross sections for electron capture from inner shells, described by the nonrelativistic screened hydrogenic wave functions and observed binding energies, to hydrogenic states of a fully stripped ion were derived, in the OBK approximation, by Nikolaev.[13] Nikolaev's cross section for electron capture from an S shell to the S' state (characterized by the quantum numbers n_2 and n_1, respectively) on the projectile of velocity v_1 is[14]

$$\sigma_{SS'}^{\rm OBK}=\frac{2^9\pi}{5}\left(\frac{n_1n_2}{v_1}\right)^2\left(\frac{v_{1S'}}{v_{2S}}\right)^5\xi_{SS'}^{10}(\theta_S)\times\frac{\Phi_4[(1-\theta_S)\xi_{SS'}^2(\theta_S)]}{[1+(1-\theta_S)\xi_{SS'}^2(\theta_S)]^3}\,, \quad (1)$$

where

$$\xi_{SS'}(\theta_S)=v_{2S}/[v_{1S'}^2+q_{SS'}^2(\theta_S)]^{1/2}. \quad (2)$$

Here,

$$q_{SS'}(\theta_S)=\tfrac{1}{2}[v_1+(v_{2S}^2\theta_S-v_{1S'}^2)/v_1] \quad (3)$$

approximates the minimum momentum transfer with $\frac{1}{2}v_{2S}^2\theta_S$ denoting the observed binding energy[15] and, $v_{2S}=Z_{2S}/n_2$ and $v_{1S'}=Z_1/n_1$ represent the orbital velocities of the electron before and after its capture, respectively. We find that in Eq. (1) the function:

$$\Phi_4[t]\equiv\frac{5}{t}\left\{1-\frac{4}{t}\left[\left(1+\frac{1}{t}\right)^3\ln(1+t)-\left(1+\frac{1}{t}\right)^2-\frac{1}{2}\left(1+\frac{1}{t}\right)-\frac{1}{3}\right]\right\} \quad (4)$$

can be approximated to within 2% by $(1+0.3t)^{-1}$ for $t<3$, i.e., for the values of t which are available in experiments.

Note that for electron capture from a hydrogenic S shell—with $\theta_S=1$, $Z_{2S}=Z_2$, and $\Phi_4[t=0]=1$—Eq. (1) reduces to the well-known OBK formula for electron transfer between hydrogenlike shells.[16] In the following, we will restrict our discussion to capture from a screened hydrogenic K shell ($n_2=1$) described by $Z_{2K}=Z_2-0.3$ and θ_K. It is interesting to observe that the ratio of cross sections for electron capture to those which are derived with the same screened hydrogenic wave functions for direct ionization is given in the limit of low projectile velocity as $(4.5/\theta_K)(Z_1/n_1Z_{2K})^3$; the contribution of electron capture to ionization is then negligible when $Z_1 \ll Z_2$ but becomes comparable to the contribution of direct ionization as Z_1/Z_2 approaches $\frac{1}{2}$. One recalls that, in the determination of ionization cross sections, electron capture to the continuum of the projectile can be neglected for all Z_1 since, as we have previously estimated,[1] the cross sections for such capture are at least $2Z_1^3$ times smaller than the cross sections for electron capture to a bound state on the projectile. Also, we would like to state that, contrary to conclusions[17] inferred from the paper of Dettmann *et al.*,[18] our estimate predicted the Z_1^2 dependence of the cross sections for electron capture to the projectile continuum; this dependence was found and confirmed in the measurements reported very recently.[17]

In the analysis of electron capture to a bound S' state on the low-velocity ion, we have accounted for the binding effect with the factor

$$\epsilon_K^B(\xi_{KS'};c_K=1.5)=1+\frac{2Z_1}{Z_{2K}\theta_K}g_K(\xi_{KS'};c_K=1.5)\,, \tag{5}$$

where g_K can be approximated [see Eq. (19) of Ref. 11], with errors less then 1%, by

$$g_K(\xi_{KS'};c_K=1.5)=(1+9\xi+31\xi^2+98\xi^3+12\xi^4+25\xi^5+4.2\xi^6+0.515\xi^7)/(1+\xi)^9\,. \tag{6}$$

The cutoff value of $c_K=1.5$ for the binding effect comes from the requirement that the increased binding due to the proximity of the projectile ion takes place only at the impact parameters which are less than the mean radius of the electron, $\langle r\rangle_K$, in the K shell.[2,10,11] The Coulomb-deflection factor is given by[1,19]

$$C=\exp[-\pi d q_{KS'}(\epsilon_K^B\theta_K)]\,, \tag{7}$$

where $d=Z_1Z_2/Mv_1^2$, with $M^{-1}\equiv M_1^{-1}+M_2^{-1}$ being the reduced mass of the scattering system, approximates the half-distance of closest approach in a head-on collision.

The cross section for low-velocity ions,

$$\sigma_{KS'}^{<}=C\cdot\sigma_{KS'}^{\rm OBK}[\xi_{KS'}(\epsilon_K^B\theta_K),\epsilon_K^B\theta_K]\,, \tag{8}$$

is joined with the cross section for high-velocity ions,[20]

$$\sigma_{KS'}^{>}=\tfrac{1}{3}\sigma_{KS'}^{\rm OBK}[\xi_{KS'}(\theta_K),\theta_K]\,, \tag{9}$$

through the expedient formula

$$\sigma_{KS'}^{\gtrless}=\sigma_{KS'}^{<}\sigma_{KS'}^{\rm OBK}/(\sigma_{KS'}^{\rm OBK}+2\sigma_{KS'}^{<})\,, \tag{10}$$

from which one easily recovers Eqs. (8) and (9) in the limits of, respectively, low and high velocity since $\sigma_{KS'}^{<}\to\sigma_{KS'}^{\rm OBK}$ as $\epsilon_K^B\to1$ and $C\to1$ when $v_1\gg v_{2K}$, and $\sigma_{KS'}^{\rm OBK}\gg\sigma_{KS'}^{<}$ when $v_1\ll v_{2K}$.

Equation (10) should be viewed only as a convenient analytical way of connection between Eqs. (8) and (9). This interpolation has no physical justification other than it happens to be in error within experimental uncertainties; in this sense Eq. (10) is semiempirical in the *intermediate*-velocity regime.

Finally, one obtains the cross section for electron capture from the K shell to all empty shells of the fully stripped ions as

$$\sigma_K=\sum_{S'}\sigma_{KS'}\simeq\sigma_{KK'}+\sigma_{KL'}+2\sigma_{KM'}\,, \tag{11}$$

since, within a few percent, $\sigma_{KS'}\simeq(3/n_1)^3\sigma_{KM'}$ for $n_1>3$ and $\sum_{n=3}^{\infty}(3/n)^3\simeq2$.

A procedure reproducing the cross sections based on relativistic wave functions has been developed in Ref. 11 for direct ionization. In this method, the electron mass $m=1$ in the nonrelativistic cross sections was replaced by its relativistic value, m_K^R, which had been found from the virial theorem and suitably averaged with the weight functions that give impact-parameter dependence for direct ionization. In an analogous manner, for electron capture we find

$$m_K^R[\xi_{KS'}(\theta_K)]=(1+1.1y_K^2)^{1/2}+y_K\,, \tag{12}$$

with

$$y_K=0.40(Z_{2K}/137)^2/\xi_{KS'}(\theta_K)\,,$$

and substitute $m_K^R[\xi_{KS'}(\theta_K)]v_1^2$ for v_1^2 in Eq. (1) to obtain $\sigma_{KS'}^{\rm OBKR}$, the cross section which should duplicate the OBK calculations based on a relativistic description of the target K shell. Note that to incorporate the relativistic effect in the present approach, the change of velocity prescribed above should be made only in the arguments of the $\sigma_{KS'}^{\rm OBK}$ function [see Eqs. (8) and (9)]; the Coulomb deflection factor comes from the description of the projectile trajectory and is essentially independent

TABLE I. Nonrelativistic and relativistic cross sections (in barns) for electron capture and quantities required for their computation. The numerical values pertain to the sample calculation delineated in the Appendix for electron capture from K shell of krypton by 26-MeV fully stripped fluorine ions.

	$^{19}_{9}F^{9+} \rightarrow {}_{36}Kr(K)$, $v_1 = 7.43$						
	Nonrelativistic			Relativistic			
Quantity	$S'=K'$ $(n_1=1)$	$S'=L'$ $(n_1=2)$	$S'=M'$ $(n_1=3)$	$S'=K'$ $(n_1=1)$	$S'=L'$ $(n_1=2)$	$S'=M'$ $(n_1=3)$	Equation
$m_K^R\,[\xi_{KS'}(\theta_K)]$	1	1	1	1.055	1.057	1.058	Eq. (12)
$q_{KS'}\ (\theta_K=0.826)$	69.1	73.2	74.0	67.5	71.4	72.1	Eq. (3)
$\xi_{KS'}\ (\theta_K=0.826)$	0.512	0.487	0.482	0.524	0.499	0.495	Eq. (2)
$\sigma_{KS'}^{OBK}\,[b]$	177	13.6	3.66	211	16.3	4.47	Eq. (1)
$\sigma_K^{OBK}\,[b]$		198			236		Eqs. (11) and (1)
$g_K\ (\xi_{KS'};c_K=1.5)$	0.694	0.717	0.721	0.694	0.717	0.721	Eq. (6)
$\epsilon_K^B\ (\xi_{KS'};c_K=1.5)$	1.424	1.438	1.440	1.424	1.438	1.440	Eq. (5)
$m_K^R\,[\xi_{KS'}(\epsilon_K^B\theta_K)]$	1	1	1	1.079	1.083	1.083	Eq. (12)
$q_{KS'}\ (\epsilon_K^B\theta_K)$	99.1	104	105	95.7	100	101	Eq. (3)
$\xi_{KS'}\ (\epsilon_K^B\theta_K)$	0.359	0.343	0.340	0.371	0.357	0.353	Eq. (2)
C	0.937	0.934	0.934	0.937	0.934	0.934	Eq. (7)
$\sigma_{KS'}^{<}\,[b]$	5.97	0.470	0.128	7.72	0.652	0.172	Eq. (8)
$\sigma_{KS'}\,[b]$	5.59	0.440	0.120	7.19	0.604	0.160	Eq. (10)
$\sigma_K\,[b]$		6.27			8.11		Eqs. (11) and (10)

of the target wave functions.[19,21]

Although the relativistic effect is insignificant for most of the available data[22-35] for relatively light target atoms, its importance might be appreciated in future experiments for the collisions of superheavy elements with slow and yet fully stripped ions. The relativistic correction according to Eq. (12) increases the cross section for electron capture from the K shell of $_{36}$Kr to the K' shell of a 26-MeV $_9F^{9+}$ by as much as ~30% (see Table I).

III. COMPARISON WITH EXPERIMENT

In Fig. 1, the cross sections for electron capture from K shells of carbon, nitrogen, oxygen, neon, and argon by protons, as they were extracted from coincidence measurements,[22] are compared with the results of OBKR [Eqs. (1) and (12)] and our calculations. The present approach gives much better agreement with the data than the OBKR approximation. Experiments in the low-velocity range (on the low-energy side of the cross-section maxima) would offer an even sharper gauge for distinction between

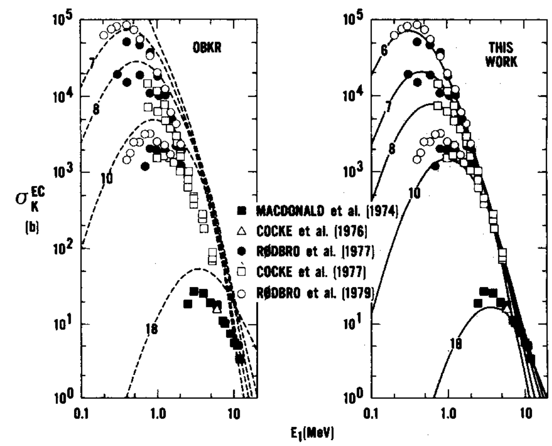

FIG. 1. Cross sections for electron capture from the K shell of $_6$C, $_7$N, $_8$O, $_{10}$Ne, and $_{18}$Ar to protons according to Eq. (11) with Eq. (1) (dashed curves) and Eq. (10) (solid curves). Both calculations account for the relativistic effect which is negligible for the target elements and proton energies shown in this figure. Data are from Ref. 22 and have uncertainties comparable to the size of the symbols.

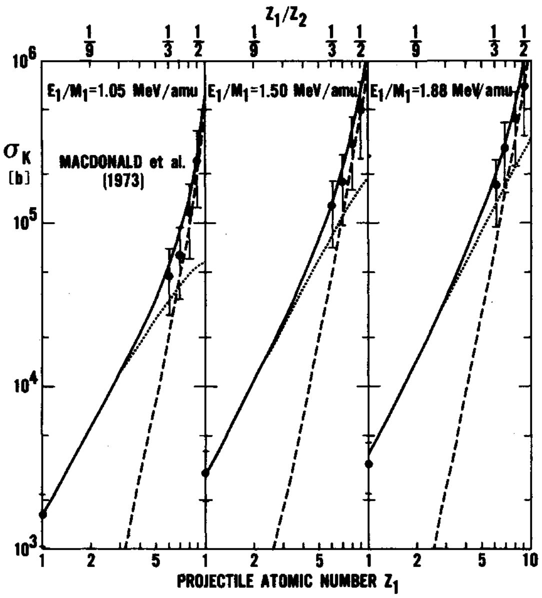

FIG. 2. Cross sections for K-shell ionization in $_{18}$Ar by fully stripped ions according to the direct ionization theory (Refs. 10 and 11) (dotted curves) and to the electron capture as given in Eqs. (10)–(12) (dashed curves). The solid curves represent the sum of direct ionization and electron capture cross sections. Data are from Ref. 24; error bars include our estimates of uncertainties in the fluorescence yields which were corrected for multiple ionization. For comparison see Fig. 4 in Ref. 1.

the predictions which start to diverge from each other by as much as an order of magnitude. The relative paucity of coincidence data for electron capture leads us to consider K-shell x-ray-production cross sections that, after division by fluorescence yields, are converted to ionization cross sections for comparison with theoretical results. Ionization cross sections are assumed to be given by the sum of electron-capture and direct-ionization cross sections. As shown in Fig. 2, excellent agreement is obtained between the data[24] and our predictions added to the results of Ref. 10 for direct ionization of the argon K shell.

Figure 3 demonstrates that agreement between the data[35] and our formulas is quite good, especially for fully stripped projectiles. The theoretical cross sections have been obtained without the use of semiempirical scaling factors for electron capture. However, for the ions with filled K' shells (closed circles) and atomic numbers $6 \le Z_1 \le 9$ the direct ionization theory[10] overestimates the data, whereas the direct ionization theory which does not account for the polarization of the target inner shell appears to coincide with experiment.[4] This observation led Gray *et al.*[4] to conclude that the direct ionization theory of Ref. 10, which includes the polarization effect, is incorrect. We would

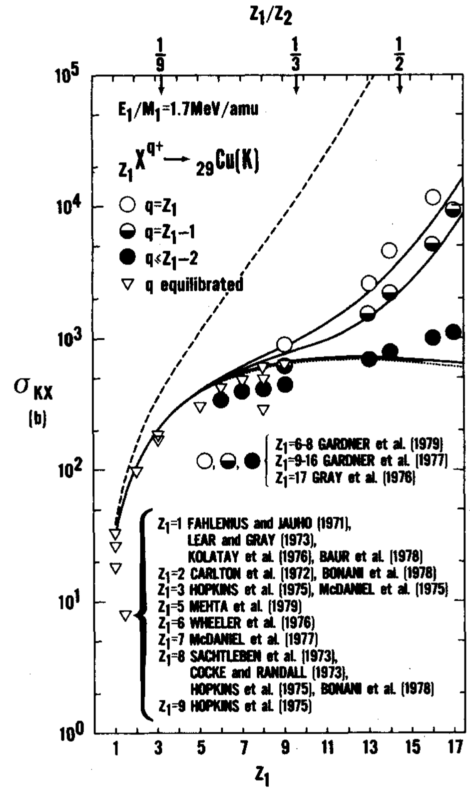

FIG. 3. Cross sections for K-shell x-ray production in $_{29}$Cu by fully stripped (○), hydrogenlike (◒), heliumlike (●), and equilibrated (▽) ions of atomic number $1 \le Z_1 \le 17$ and same velocity $E_1 M_1 = 1.7$ MeV/amu. The dotted curve is based on the direct ionization calculations of Refs. 10 and 11. The solid curves are obtained after the addition of electron-capture cross sections of Eqs. (10)–(12) for fully stripped, hydrogenlike and heliumlike charge states of the projectile. The dashed curve represents the sum of the first Born approximation with the relativistic effect in the plane-wave Born approximation relativistic wave functions (PWBAR) calculations for direct ionization and the OBKR results, Eqs. (1), (11), and (12), for electron capture by fully stripped projectiles. Data are from Ref. 35 and have uncertainties comparable to the size of the symbols; the cross sections for the equilibrated ions with Z_1=1, 2, 3, 4, 5, 6, 8, and 9 were obtained from Ref. 35 either directly or through interpolation (see Ref. 37). The fluorescence yield ω_K= 0.44 was used as recommended in Ref. 38.

like to point out that the theory was developed for fully stripped ions; the screening of the high-velocity projectile by its electrons results in smaller direct ionization cross sections which may explain the observed discrepancy.[36] Concurrently, the orbital velocities of K' shell electrons for the $13 \le Z_1 \le 17$ ions are larger than $v_1 = 8.3$, i.e., these ions are slow enough for the adiabatic adjustment of their innermost electrons which may, via their increased binding energy in the presence of the target nucleus, enlarge the electron-capture channel for ionization.

We would further like to emphasize the importance of comparing experimental data to the appropriate theoretical calculations. For collision systems, such that $Z_1/Z_2 \gtrsim 1/4$, the contributions of electron capture to target ionization must be considered. These contributions are present when inner-shell vacancies are created in the ion before the collision either by prior preparation of the ion or by multiple encounters in the target. For target thickness of a few hundred $\mu g/cm^2$, the ions approach a charge-state equilibrium and may possess a number of inner-shell vacancies.[2,4] In Fig. 3 we have added cross sections for ions in equilibrated charge states.[35] For $Z_1/Z_2 \lesssim 1/4$ the electron-capture contributions to ionization are only a few percent and the equilibrated data are in good agreement with the nonequilibrated data as well as the theoretical calculations.

A comparison, in Fig. 4, for K-shell x-ray production in various targets lighter than copper by 1.7-MeV/amu fluorine ions reveals an excellent agreement between results of the calculations and the data[4,30,33,34] when the targets of $Z_2 \leq 26$ are bombarded by heliumlike $_9$F ions and, therefore, appears to contradict the inferences about the importance of the screening effect that we have made in the discussion of Fig. 3. It should be noted, however, that the calculated ionization cross sections were converted to x-ray-production cross sections through multiplication by the fluorescence yields[38] which were not corrected for multiple ionizations. These ionizations might, via larger yields, increase the calculated x-ray-production cross sections in such a manner as to fortuitously offset their decrease due to the screening effect. The corrected fluorescence yields become significantly larger than those of Ref. 38 when Z_2 decreases; in particular, such increases could be very dramatic for $Z_1/Z_2 \geq \frac{1}{3}$ in Fig. 4 as opposed to the collision systems with $Z_1/Z_2 < \frac{1}{3}$ in Fig. 3 for which the discrepancy between the theory and experiment may be a genuine measure of the screening effect in ionization by heliumlike projectiles.

For $Z_1/Z_2 \geq \frac{1}{2}$ the predictions of the present approach which strictly applies in the $Z_1 \ll Z_2$ limit, tend to overestimate[39] the measurements as exhibited. Figure 5 and Table II show the ratios of theoretical and experimental[2,4,23-34] cross sections for K-shell x-ray production by fully stripped ions. However, for $Z_1/Z_2 < \frac{1}{2}$ these ratios are predominantly well within a factor of 2 of the ideal ratio

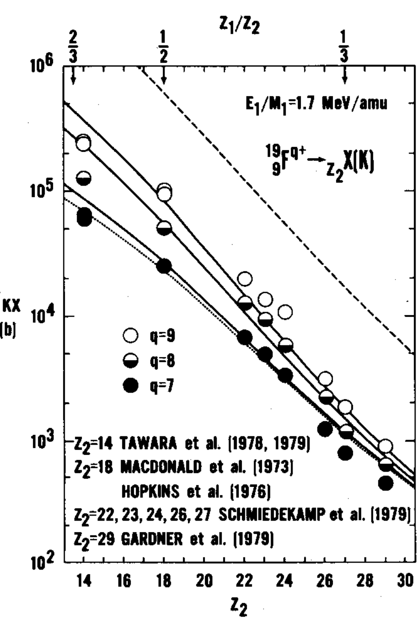

FIG. 4. Cross sections for K-shell x-ray production in the targets of atomic number $14 \leq Z_2 \leq 29$ by 1.7-MeV $_9F^{9+}$ (○), $_9F^{8+}$ (◒), and $_9F^{7+}$ (●) ions. The meaning of the curves is the same as in Fig. 3. Data are from Refs. 4, 30, 33, and 34, and have uncertainties comparable to the size of the symbols; the fluorescence yields were used as given in Ref. 38.

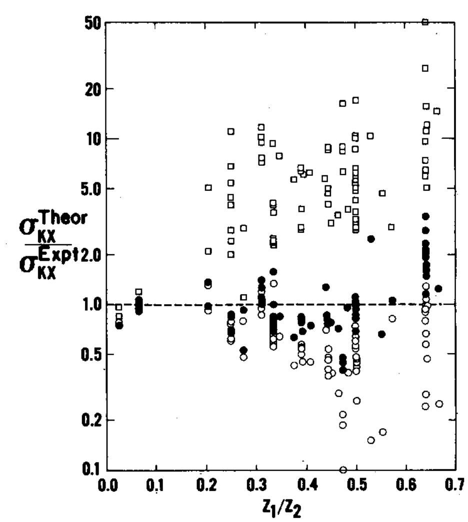

FIG. 5. Ratios of the theoretical σ_{KX}^{Theor} and experimental (Refs. 2, 4, and 26–34) σ_{KX}^{Expt} cross sections for K-shell x-ray production by fully stripped ions. To obtain σ_{KX}^{Theor}, the calculated K-shell ionization cross sections were multiplied by the fluorescence yields of Ref. 38. Symbols represent the ratios found with different calculations: first Born approximation (□) and the Coulomb-deflected perturbed-stationary-state relativistic (CPSSR) theory of direct ionization (Refs. 10 and 11) plus electron capture according to Ref. 1 (○) or plus electron capture according to this work, Eqs. (10)–(12) (●).

TABLE II. The ratios of theoretical and experimental cross sections for K-shell x-ray production by fully stripped ions versus Z_1/Z_2 as plotted in Fig. 5. The theoretical cross sections for ionization, obtained from the CPSSR theory of direct ionization (Refs. 10 and 11) and present work for electron capture, were multiplied by the fluorescence yields of Ref. 38.

Z_1/Z_2	$\sigma_{KX}^{\text{Theor}}/\sigma_{KX}^{\text{Expt}}$	E_1/M_1 (MeV/amu)	Reference to $\sigma_{KX}^{\text{Expt}}$ and (Z_1, Z_2)	Z_1/Z_2	$\sigma_{KX}^{\text{Theor}}/\sigma_{KX}^{\text{Expt}}$	E_1/M_1 (MeV/amu)	Reference to $\sigma_{KX}^{\text{Expt}}$ and (Z_1, Z_2)
0.028	0.73	1.89	28 (1, 36)		0.82, 0.80	1.50	
	0.77	2.53			0.86, 0.87	1.88	
	0.73	3.00		0.448	0.76	1.71	32 (13, 29)
0.056	0.93	1.05	24 (1, 18)	0.472	0.41	2.86	29 (17, 36)
	1.03	1.50			0.22	3.43	
	1.05	1.88			0.46	4.00	
	1.03	1.05			0.45	4.57	
	1.01	1.58		0.483	0.71	1.71	32 (14, 29)
	0.99	1.87			0.96	1.86	2 (14, 29)
	0.93	1.89	28 (1, 18)	0.500	0.93, 0.88	1.88	23 (9, 18)
	0.96	2.53			0.70, 0.69	1.05	24 (9, 18)
	0.95	3.00			0.82, 0.84	1.50	
	0.90	2.00	31 (1, 18)		1.04	1.89	28 (9, 18)
0.205	1.38	3.00	27 (8, 39)		0.93	2.53	
	0.97	5.00			1.15	1.05	30 (9, 18)
0.250	0.83	1.89	28 (9, 36)		0.98	1.37	
	0.80	2.53			1.00	1.63	
	0.85	1.37	30 (9, 36)		1.15	1.89	
	0.65	1.89			1.14	2.16	
	0.70	2.42			1.01	2.42	
	0.64	2.95			1.01	2.68	
	0.65	3.47			0.96	2.95	
	0.64	4.00			0.97	3.21	
0.276	0.92	3.00	27 (8, 29)		1.01	3.47	
	0.52	5.00			1.05	3.74	
0.310	1.11	1.71	32 (2, 29)		1.05	4.00	
	1.01	1.70	4 (2, 29)		0.88	1.58	31 (9, 18)
	1.18	2.00		0.529	2.52	2.26	26 (9, 17)
	1.26	2.25		0.552	0.67	1.71	32 (16, 29)
	1.40	2.5		0.571	1.07	2.50	25 (18, 14)
0.333	0.78, 0.75	1.05	24 (6, 18)	0.636	1.17	1.86	2 (14, 22)
	0.70, 0.76	1.50		0.643	3.40	0.40	32 (9, 14)
	0.85, 0.80	1.88			3.20	1.60	
	1.58	2.5	31 (6, 18)		2.80	0.80	
0.333	1.00	1.70	4 (9, 27)		2.36	1.00	
0.346	0.85	1.70	4 (9, 26)		2.17	1.20	
0.375	0.63	1.70	4 (9, 24)		2.08	1.40	
0.389	0.84, 0.78	1.05	24 (7, 18)		1.82	1.60	
	0.79	1.50			1.73	1.80	
	0.80, 0.78	1.88			1.79	2.00	
	0.84	1.59			1.91	2.20	
0.391	0.69	1.7	4 (9, 23)		1.62	1.00	34 (9, 14)
0.409	0.74	1.7	4 (9, 22)		1.48	2.00	
0.438	1.27	1.86	2 (14, 32)	0.667	1.27	1.86	2 (14, 21)
0.444	0.79, 0.74	1.05	24 (8, 18)				

of unity once the theory follows the present treatment for electron capture (closed circles). By contrast, the first Born approximation with OBKR cross sections of Nikolaev for electron capture (squares) leads to the K-shell ionization cross sections which, with increasing Z_1/Z_2, can be larger than the experimental values by more than one order of magnitude. The open circles represent the ratios obtained with the full binding effect as described in Ref. 1.

IV. SUMMARY

We have demonstrated that the cross sections for electron capture and ionization, as inferred from data for K-shell x-ray production by fully stripped ions, can be accurately predicted without a recourse to semiempirical scaling factors. The calculations, which are cast in terms of the well-known OBK formulas of Nikolaev and performed analytically, may obviate the persistent attempts that scale the OBK cross sections empirically. This work summarizes the previous development of an analytical approach for electron capture[1,2] and extends it to incorporate the relativity effect in a manner analogous to the procedure formulated recently for direct ionization.[11]

We point to difficulties in analysis of the data obtained with nonfully stripped ions; subtle differences between various approaches in the theory for direct ionization, which was developed for fully stripped projectiles, cannot and should not be assessed by comparison with such data. One notes that, aside from relatively large experimental uncertainties, a theoretical problem arises as to the role of the electrons on the projectile. Beyond mere determination of its charge state, these electrons result in a delicate balance between the opposing effects of screening and binding on the projectile. A rigorous treatment of these effects is outside the scope of the present work.

This work is in good agreement with the vast amount of data for fully stripped ions when $Z_1/Z_2 < \frac{1}{2}$. Still, we would like to reiterate the need for more direct measurements for electron capture by low-velocity projectiles, and for, if supplemented by reliable fluorescence yields, more x-ray experiments in the $Z_1/Z_2 > 0.3$ collision systems with gaseous or vanishingly thin solid targets and fully stripped projectiles. Such experiments will further test the limits of applicability of the present formulas which, judging from Fig. 5, start to overestimate the data when $Z_1/Z_2 \geq \frac{1}{2}$. Ultimately, this perturbative approach should be scrutinized by the results of numerical coupled-state calculations; in particular, such calculations may test the validity of the assumption that ionization cross sections are simply given as a sum of the cross sections for direct ionization and electron capture. A comparison between our formulas and results of a more advanced numerical calculation should be beneficial for both approaches; such a comparison may serve as a guide in the development of a rigorous theory and, simultaneously, it should resolve the question of validity and limitations of the present approach.

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APPENDIX: SAMPLE CALCULATIONS OF CROSS SECTIONS FOR ELECTRON CAPTURE

We illustrate the scheme of cross section calculations for electron capture from the K shell of argon ($Z_2=18$, $M_2=39.95$ amu$=39.95\times 1823$, $v_{2K}=Z_{2K}=17.7$, $\theta_K=0.751$) to all shells of 10-MeV protons ($Z_1=1$, $M_1=1.007$ amu, $v_{1S}=1/n_1$) and 20-MeV fluorine ions ($Z_1=9$, $M_1=19.0$ amu, $v_{1S}=9/n_1$) which, respectively, are the ions of high ($v_1=20.1$, $v_1/v_{2K}=1.136$) and low ($v_1=6.51$, $v_1/v_{2K}=0.368$) velocity in comparison with the orbital velocity of the K-shell electrons in ${}_{18}$Ar. The velocity v_1 is given in atomic units by $v_1=6.35(E_1/M_1)^{1/2}$ if E_1/M_1 is expressed in MeV/amu. In Table III we present the numerical values of the electron capture cross sections and quantities required for their computation for the electron capture from the K shell of Ar by 10-MeV protons and 20-MeV fluorine ions.

Since Eq. (1) is written in atomic units of $a_0^2=2.8\times 10^7$ b it reads in barns as

$$\sigma_{KS'}^{\mathrm{OBK}}[\xi_{KS'}(\theta_K),\theta_K]=9\times 10^9\ \mathrm{b}\left(\frac{Z_1}{Z_{2K}}\right)^5\frac{\xi_{KS'}^{10}(\theta_K)}{v_1^2 n_1^3}\times\frac{[1+0.3(1-\theta_K)\xi_{KS'}^2(\theta_S)]^{-1}}{[1+(1-\theta_K)\xi_{KS'}^2(\theta_K)]^3}, \quad \text{(A1)}$$

and, for the capture from the K shell of argon, further simplifies to

$$\sigma_{KS'}^{\mathrm{OBK}}[\xi_{KS'}(\theta_K),\theta_K]=5180\ \mathrm{b}\,\frac{Z_1^5}{v_1^2 n_1^3}\,\xi_{KS'}^{10}(\theta_K)\times\frac{[1+0.3(1-\theta_K)\xi_{KS'}^2(\theta_S)]^{-1}}{[1+(1-\theta_K)\xi_{KS'}^2(\theta_K)]^3}, \quad \text{(A2)}$$

where

$$\xi_{KS'}(\theta_K)=17.7/[Z_1^2/n_1^2+q_{KS'}^2(\theta_K)]^{1/2}, \quad \text{(A3)}$$

with

$$q_{KS'}(\theta_K)=\tfrac{1}{2}\left(v_1+\frac{313.3\theta_K-Z_1^2/n_1^2}{v_1}\right). \quad \text{(A4)}$$

The binding effect is accounted for with the factor [see Eqs. (5) and (6)]

$$\epsilon_K^B(\xi_{KS'};c_K=1.5)=1+0.15\times Z_1\times g_K(\xi_{KS'};c_K=1.5), \quad \text{(A5)}$$

the Coulomb-deflection factor is determined with

TABLE III. Electron-capture cross sections (in barns) and quantities required for their computation. The numerical values pertain to the sample calculations delineated in the Appendix for electron capture from the K shell of argon by 10-MeV protons and by 20-MeV fully stripped fluorine ions.

Quantity	$^{1}_{1}H^{+} \to {}_{18}Ar(K)$ $v_1 = 20.0$ $S' = K'$ $(n_1 = 1)$	$v_1/v_{2K} = 1.130$ $S' = L'$ $(n_1 = 2)$	$S' = M'$ $(n_1 = 3)$	$^{19}_{9}F^{9+} \to {}_{18}Ar(K)$ $v_1 = 6.51$ $S' = K'$ $(n_1 = 1)$	$v_1/v_{2K} = 0.368$ $S' = L'$ $(n_1 = 2)$	$S' = M'$ $(n_1 = 3)$	Equation
$g_{KS'}$ $(\theta_K = 0.751)$	15.9	15.9	15.9	15.1	19.8	20.6	Eqs. (3) and (A4)
$\xi_{KS'}$ $(\theta_K = 0.751)$	1.111	1.113	1.113	1.007	0.872	0.850	Eqs. (2) and (A3)
$\sigma_{KS'}^{\mathrm{OBK}}$ [b]	15.2	1.93	0.572	3.66×10^{6}	1.28×10^{5}	3.04×10^{4}	Eqs. (1) and (A2)
$\sigma_{K}^{\mathrm{OBK}}$ [b]		18.3			3.85×10^{6}		Eqs. (11) and (1)
g_K $(\xi_{KS'};c_K = 1.5)$	0.304	0.303	0.303	0.350	0.421	0.435	Eq. (6)
ϵ_K^B $(\xi_{KS'};c_K = 1.5)$	1.406	1.046	1.046	1.473	1.568	1.587	Eqs. (5) and (A5)
$g_{KS'}$ $(\epsilon_K^B\theta_K)$	16.1	16.1	16.1	23.7	30.0	31.2	Eq. (3)
$\xi_{KS'}$ $(\epsilon_K^B\theta_K)$	1.097	1.099	1.099	0.698	0.583	0.565	Eq. (2)
C	0.999	0.999	0.999	0.998	0.985	0.984	Eq. (7)
$\sigma_{KS'}^{<}$ [b]	15.2	1.93	0.573	2.33×10^{5}	4.95×10^{3}	1.07×10^{3}	Eq. (8)
$\sigma_{KS'}$ [b]	5.07	0.643	0.191	2.07×10^{5}	4.59×10^{3}	1.00×10^{3}	Eq. (10)
σ_K [b]		6.10			2.14×10^{5}		Eqs. (11) and (10)

TABLE IV. Comparison of theoretical and experimental cross sections (in barns). For each collision system, the first Born approximation results [PWBAR for direct ionization and OBKR of Eqs. (1) and (12) for electron capture] and the predictions of the CPSSR theory, of Refs. 10 and 11 for direct ionization and present work [see Eq. (11) with Eq. (10)] for electron capture, are compared to the experimental data. Evaluation of electron capture cross sections is made in Tables III (for argon without the relativistic effect) and I (for krypton with the relativistic effect). The fluorescence yields are from Ref. 38.

Collision system	Direct ionization (PWBAR) + Electron capture (OBKR) = Ionization	Direct ionization (CPSSR) + Electron capture (Present work) = Ionization	Experimental data
${}_{1}H^{+} \to {}_{18}Ar(K)$ $E_1 = 10$ MeV (electron capture only)	18.1	6.10	5.6 Macdonald *et al.* (1974) (see Ref. 22)
${}_{9}F^{9+} \to {}_{18}Ar(K)$ $E_1 = 20$ MeV $\omega_K = 0.118$	$0.15\times10^{6} + 3.85\times10^{6} = 4.0\times10^{6}$	$0.53\times10^{5} + 2.14\times10^{5} = 2.67\times10^{5}$	3.9×10^{5} Macdonald *et al.* (1973) (see Ref. 24) 2.7×10^{5} Hopkins *et al.* (1976) (see Ref. 30)
${}_{9}F^{9+} \to {}_{36}Kr(K)$ $E_1 = 26$ MeV $\omega_K = 0.643$	544 + 236 = 780	52.1 + 8.11 = 60.2	70 Hopkins *et al.* (1976) (See Ref. 30)

$q_{KS'}(\epsilon_K^B\theta_K)$ of Eqs. (A4) and (A5), and

$$d=\frac{Z_1\times 18\times (M_1+39.95)}{M_1\times 39.95\times 1823\times v_1^2},$$

so that $d=0.000\,163$ for 20-MeV ${}^{19}_{9}F^{9+}$ and $d=0.000\,025$ for 10-MeV ${}^{1}_{1}H^{+}$.

The relativistic effect can be neglected since even for the slower fluorine ions in our calculation, the relativistic mass m_K^R is, by Eq. (12), $\lesssim 1\%$ larger than its nonrelativistic value in the K shell of argon. For electron capture from the K shell of krypton ($Z_2=36$, $M_2=83.8$, $V_{2K}=Z_{2K}=35.7$, $\theta_K=0.826$) by relatively slower ($v_1=7.43$, $v_1/v_{2K}=0.208$) 26-MeV fluorine ions, however, the relativistic effect is significant as demonstrated in Table I. Table I presents nonrelativistic and relativistic cross sections for electron capture and quantities required for their computation for electron capture from the K shell of krypton by 26-MeV fully stripped fluorine ions. In the nonrelativistic columns, m_K^R is equal to 1 in atomic units of mass by definition. In the relativistic calculations m_K^R, g_K, and ϵ_K^B are evaluated for the nonrelativistic values of ξ_K.

The results of our sample calculations are summarized and compared with available data[22,24,30] in Table IV. The values exhibited in Table I and III for intermediate quantities in evaluation of cross sections may differ in the last digit from the actual values due to round-off errors.

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[39]This theory was developed in the prior formulation with the projectile perturbing the initial state of the electron on the target; in the $Z_1 \gg Z_2$ limit the post approach with the target perturbing the final state of the electron on the projectile should be employed. When $Z_1/Z_2 \to 1$ some symmetrized version of both formulations ought to apply and result in *larger* cross sections than either one of these approaches because of the cancellation of the binding effects.