

Electron capture from inner shells by fully stripped ions*

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Cross sections for electron capture from inner atomic shells by fully stripped ions, of velocities high compared to the electron velocities in the inner-shell orbits, are calculated in the second Born approximation. The theory of Drisko for electron capture by protons from hydrogen is generalized to projectiles and targets of arbitrary atomic numbers Z_1 and Z_2 , respectively. For ions of low velocity, the effects of binding and Coulomb deflection are accounted for in a manner similar to that of Brandt and his co-workers in the theory for direct ionization to the continuum of the target atom. The results are in good agreement with experimental capture cross sections, whereas the Oppenheimer-Brinkman-Kramers approximation overestimates such cross sections. The contribution of electron capture to inner-shell ionization cross sections increases with increasing Z_1/Z_2 and brings them into agreement with experiment.

I. INTRODUCTION

Over the last few years, it has become apparent that ionization of a target atom by a moving charged particle proceeds not only through direct ionization to the continuum of the target but also through electron capture by the projectile.¹⁻²² Reliable cross sections for electron capture are needed to know the contribution of this process to the creation of a vacancy in the inner shell of the target atom.²³ In the following we restrict the discussion to nonrelativistic projectiles. Then one has to consider only nonradiative electron capture, because radiative capture can be neglected.²⁴ The Oppenheimer²⁵-Brinkman-Kramers²⁶ (OBK) approximation is known to overestimate electron capture cross sections, especially for slow collisions. Nikolaev²⁷ introduced scaling factors to obtain an empirical fit for the total electron capture from all shells of the target atom. Following this idea, Halpern and Law³ proposed that the proper cross sections for electron capture from inner shells by fully stripped ions can be obtained by scaling down the OBK cross sections with an empirically fitted factor for each velocity of the projectile. Usage of an empirical "correction" has by now become a common procedure.^{6, 9, 10, 13, 17-22, 28}

We formulate the theory in a manner which does not require the introduction of such empirical correction factors. The electron-capture cross sections are derived for fully stripped ions which are either fast or slow when compared with the electron velocities in the inner-shell orbits. The calculation is as easy as the OBK approximation which is discussed in Sec. II. Section III contains the results of the second Born approximation in the high velocity limit; in Sec. IV the binding and Coulomb-deflection effects are incorporated into the theory as derived in the low-velocity limit.

The fast- and slow-collision cross sections are joined through a simple interpolation formula and compared with data in Sec. V. Appendix A gives impact-parameter-dependent functions for electron capture as calculated in the OBK approximation and utilized in the derivation of the binding effect. A sample calculation of electron-capture cross sections is delineated in Appendix B.

Except in the figures, atomic units are used throughout.

II. OBK APPROXIMATION

Theories of electron capture have been summarized in numerous books and review articles.²⁹⁻³⁸ Only a concise set of facts about the OBK approximation as it pertains to our approach is presented in this section. We consider the electron capture from an inner shell $S=K, L$, or subshell $S=K, L_1, L_2, L_3$ of the target atom to a bound (S' shell) or a continuum state of the fully stripped ion. Such a rearrangement collision can be reduced to a three-body scattering problem by the active-electron assumption,³⁷ viz., that all electrons, except for the one which is being transferred, are passive spectators in the collision. Their function is to screen (i) the active electron from its target nucleus, and (ii) the Coulomb repulsion between the nuclei of the target atom and projectile.

The role of the internuclear interaction has been treated extensively in the literature, often as a controversy. The neglect of this interaction in the perturbing potential of the first plane-wave Born approximation is known as the OBK approximation. We summarize the arguments in support of this approximation. On physical grounds, cross sections should not be changed by simply adding a constant in the perturbing potential.²⁵ The internuclear interaction is such a constant with respect

to the electronic variables. The neglect of the internuclear interaction between the projectile-target nuclei, of mass M_1 , $M_2 \gg 1$, was justified rigorously in the high-velocity limit.^{39,40} A first-order solution of coupled equations for the transition amplitudes is possible for all velocities after a canonical transformation (see, e.g., p. 200 of Ref. 34) which moves the internuclear interaction into a phase factor.⁴¹ Except for electron capture by protons from hydrogen,^{42,43} the first plane-wave Born approximation grossly overestimates the experimental cross sections.^{44,45} The reduction of the internuclear interaction, in such a way as to make the total perturbing potential vanish at infinite separations,⁴⁶ does not seem to give much of an improvement over the OBK approximation.

A. Electron capture to bound states

The OBK calculations for electron transfer between the ground states of the hydrogen-proton system^{25,26} have been extended to first excited states,⁴⁷ and to all possible rearrangements between the states of hydrogenlike atoms.⁴⁸⁻⁵¹ The sum rules for the Fourier transforms of the hydrogenic states lead to the simple result that the cross section for electron capture by the particle of velocity v_1 is⁵²

$$\sigma_{SS'}^{\text{OBK}} = \frac{2^9 \pi n_1^2}{5 v_1^2} \left(\frac{v_{1S} v_{2S}}{v_{1S}^2 + \frac{1}{4}(v_1^2 + v_{2S}^2 - v_{1S'}^2)/v_1^2} \right)^5 \quad (1)$$

in terms of the hydrogenic orbital velocities $v_{2S} = Z_2/n_2$ and $v_{1S} = Z_1/n_1$, where n_2 and n_1 are the principal quantum numbers of electrons in the S and S' shell, respectively. The OBK cross sections for subshell transitions have been derived in closed forms.⁵¹

Furthermore, the formulas based on the screened hydrogenic wave functions and observed binding energy $\frac{1}{2} v_{2S}^2 \theta_S$, were derived by Nikolaev²⁷ in the OBK approximation. We will use and denote these cross sections as $\sigma_{SS'}^{\text{OBK}}(\theta_S)$. Note that now $v_{2S} = Z_{2S}/n_2$, where $Z_{2K} = Z_2 - 0.3$ and $Z_{2L_i} = Z_2 - 4.15$ ($i = 1, 2, 3$) as prescribed by the Slater rules.⁵³ However, the projectile wave functions and energies are still hydrogenic, which restricts our considerations to fully stripped ions.

B. Electron capture to the continuum

Experiments⁵⁴⁻⁵⁹ and calculations^{57,60,61} have shown that the differential cross section for electron capture to the continuum of the projectile peaks at $\vec{k}' = \vec{k} - \vec{v}_1 = 0$, where \vec{k}' and \vec{k} are the momenta of the captured electron relative to the projectile and target atom, respectively. We have calculated this cross section in the OBK approximation and $\vec{k} - \vec{v}_1 \rightarrow 0$ limit. By integrating it over

all \vec{k}' space, one obtains an upper estimate for the electron-capture cross section to the continuum $\sigma_{\text{SC}}^{\text{OBK}}$. We find that

$$\sigma_{\text{SC}}^{\text{OBK}} = \frac{\sigma_{\text{SK}}^{\text{OBK}}}{2Z_1^3} \left\{ \frac{[v_1 + (v_{2S}^2 - v_{1K}^2)/v_1]^2 + 4v_{1K}^2}{(v_1 + v_{2S}^2/v_1)^2} \right\}^5 \quad (2)$$

The expression in the braces becomes ≈ 1 in the limits of low and high velocities or when $v_{2S} \gg v_{1K}$. The cross section for electron capture to the continuum is then at least $2Z_1^3$ times smaller than $\sigma_{\text{SK}}^{\text{OBK}}$, the cross section for electron capture to a K shell. We neglect its contribution in the following.

III. HIGH-VELOCITY IONS

In an unpublished, yet well publicized^{29,32-38} thesis, Drisko⁶² derived cross sections for electron capture from hydrogen by protons of velocity $v_1 \gg 1$ as

$$\sigma(v_1 \gg 1) = (0.295 + 5\pi v_1/2^{12}) \sigma^{\text{OBK}}(v_1 \gg 1), \quad (3)$$

where $\sigma^{\text{OBK}}(v_1 \gg 1)$ denotes the OBK cross section in the high-velocity limit. Drisko's choice of particular transition amplitudes has been justified through the iteration of Faddeev's equations⁶³ as well as from the standpoint of field theory.⁶⁴ As shown by Dettmann and Leibfried,³³ Eq. (3) is obtained in the second Born approximation from

$$\frac{\sigma(v_1 \gg 1)}{\sigma^{\text{OBK}}(v_1 \gg 1)} = \int_{b_0}^{\infty} \frac{db}{b^4} \left| \frac{1}{b_c - b + i\beta_0} - \frac{1}{b} \right|^2 / \int_{b_0}^{\infty} \frac{db}{b^6}, \quad (4)$$

which, with⁶⁵ $b_c \approx 4b_0$ and after straightforward calculations,⁶⁶ leads to

$$\frac{\sigma(v_1 \gg 1)}{\sigma^{\text{OBK}}(v_1 \gg 1)} = 1 - \frac{275}{384} + \frac{5 \ln 3}{512} + \frac{5\pi b_0^2}{2^8 \beta_0}, \quad (5)$$

where $b_0^2/\beta_0 = v_1/2^4$.

We generalize this result to electron capture from an inner subshell S. The ion velocity v_1 is taken to be large compared to the velocities v_{2S} and $v_{1S'}$ of the electron in the target atom subshell and the ion shell S' before and after the collision, respectively. By inspection of Dettmann's formulas^{33,36} one notes that

$$b_0^2/\beta_0 = v_1/2^3(v_{1S'} + v_{2S}) \quad (6)$$

in Eq. (5). Thus we obtain the equation⁶⁷

$$\frac{\sigma(v_1 \gg v_{2S}, v_{1S'})}{\sigma^{\text{OBK}}(v_1 \gg v_{2S}, v_{1S'})} = 0.295 + \frac{5\pi v_1}{2^{11}(v_{1S'} + v_{2S})}. \quad (7)$$

Although derived for $v_1 \gg v_{2S}$, we extend this result to $v_1 \gtrsim v_{2S}$ to cover the experimental range $1 \lesssim v_1/v_{2S} \lesssim 10$. We use Nikolaev's OBK cross sections without going to the high- v_1 limit⁶⁸ and

obtain

$$\sigma(v_1 \geq v_{2S}, v_{1S'}) = \frac{1}{3} \sigma_{SS'}^{\text{OBK}}(\theta_S), \quad (8)$$

where the factor $\frac{1}{3}$ approximates the right-hand side of Eq. (7) to within 10% up to $v_1/v_{2S} \approx 10$.

For higher ion velocities, relativistic effects in electron capture may introduce corrections to the nonrelativistic OBK cross sections that are of comparable order to the second term in Eq. (7). In fact, the relativistic effects lower $\sigma_{SS'}^{\text{OBK}}$ by 3% for electron capture from hydrogen by 10-MeV protons⁶⁹; this happens to compensate the contribution of the second term in Eq. (7) in such a way that Eq. (8) becomes accurate with error less than 1%.

IV. LOW-VELOCITY IONS

As was done in the theory for direct ionization to the continuum of the target atom,⁷⁰⁻⁷² we include in the theory for electron capture two effects not contained in the OBK approximation. They are (i) the increase in the binding energy of the inner-shell electrons to be captured owing to the presence of the slow ion inside the inner shell during the collision (see Sec. IV A); (ii) the deflection of the ion from its initial straight-line trajectory into a Kepler orbit by the Coulomb field of the target nucleus (see Sec. IV B).

A. Binding effect

The influence of the projectile on the initial state of the electron in the low-velocity regime $v_1 \ll v_{2S}$ has been derived in the perturbed-stationary-state (PSS) theory.⁷³ We incorporate this influence in first-order perturbation theory as an effective increase of the binding energy of the electron to be captured. The first-order perturbation approach is sufficient for the capture from the innermost shells in such collision systems that $Z_1 \ll Z_2$. As prescribed by the PSS theory, the factor by which the reduced binding energy θ_S is increased

$$\hat{\epsilon}_S = 1 + \frac{1}{\frac{1}{2}v_{2S}^2\theta_S} \int d^3r \psi_S^*(\vec{r}) \frac{Z_1}{|\vec{R}_0 - \vec{r}|} \psi_S(\vec{r}) \quad (9)$$

is evaluated at the closest internuclear distance R_0 . In the straight-line trajectory approximation, R_0 equals the impact parameter p . With screened hydrogenic wave functions ψ_S and $y \equiv Z_2 p$, one obtains⁷¹

$$\hat{\epsilon}_K(y) = 1 + \frac{2Z_1 Z_{2K}}{v_{2K}^2 \theta_K} \frac{1 - e^{-2y}(1+y)}{y} \quad (10)$$

and⁷²

$$\hat{\epsilon}_{L_i}(y) = 1 + \frac{2Z_1 Z_{2L}}{v_{2L_i}^2 \theta_{L_i}} \frac{1 - e^{-y}(1 + \frac{3}{4}y + \frac{1}{4}y^2 + \frac{1}{72}c_{L_i} y^3)}{y}, \quad (11)$$

where c_{L_i} takes the values 9 and 3 for the L_1 and $L_{2,3}$ subshells, respectively.⁷⁴ We average $\hat{\epsilon}_S$ over all impact parameters⁷⁵

$$\epsilon_S = \int_0^\infty \hat{\epsilon}_S \left(\frac{x_{SS'} n_2 v_{2S}}{\sqrt{\beta}} \right) W_{SS'}(x_{SS'}) x_{SS'} dx_{SS'}, \quad (12)$$

where $x_{SS'} \equiv p\sqrt{\beta}$ with β as introduced in Appendix A. The weight functions $W_{SS'}$ correspond to W_S , the squared absolute values of the Bang-Hansteen-Mosebekk⁷⁶ matrix elements for direct ionization,⁷² and are normalized so that

$$\int_0^\infty W_{SS'}(x) x dx = 1.$$

Equation (12) can be written as

$$\epsilon_S = 1 + (2Z_1/Z_{2S}\theta_S)g_S. \quad (13)$$

When screened hydrogenic wavefunctions are employed as is done here, the $W_{SS'}$ functions are given as a combination of Bessel functions which formally differs from W_S for direct ionization (see Appendix A). However, we find this difference to be small, especially when the results of integrations in Eq. (12) with these weight functions are considered (see Fig. 1). Thus, with the analytical approximations to W_S as given in Appen-

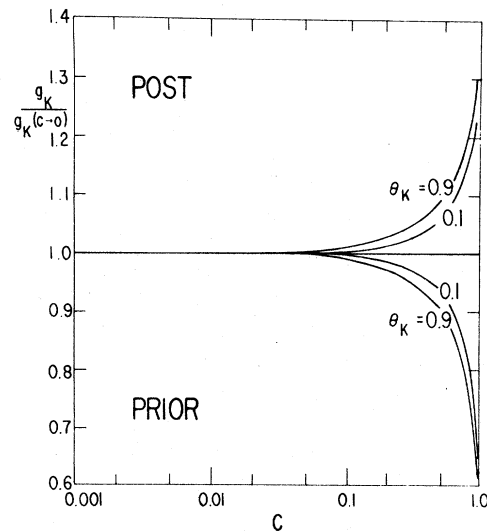


FIG. 1. Function g_K , Eq. (13), evaluated from Eq. (12) with the screened hydrogenic $W_{KK'}$, Eq. (A8), and normalized to $g_K(c \rightarrow 0)$ obtained with $W_{KK'}$ ($c \rightarrow 0$) of Eq. (A9). As defined in Appendix A, c is typically less than $\frac{1}{3}$ and proportional to v_1^2 at low velocities. Results of post and prior formulations are shown in the upper- and lower-halves of the figure, respectively.

dixes A of Ref. 72 and of this paper, one obtains

$$g_K(x) = \frac{1 + 5x + 7.14x^2 + 4.27x^3 + 0.95x^4}{(1+x)^5}, \quad (14)$$

$$g_{L_1}(x) = (1 + 7x + 15.3x^2 + 29.2x^3 + 26.7x^4 + 11.4x^5 + 1.90x^6)/(1+x)^7, \quad (15)$$

$$g_{L_{2,3}}(x) = (1 + 9x + 36x^2 + 84x^3 + 112x^4 + 89.8x^5 + 43.7x^6 + 12x^7 + 1.42x^8)/(1+x)^9, \quad (16)$$

as suitable analytical approximations to the exact functions from which g_S can be calculated with errors $\leq 1\%$.⁷⁷ Here x equals $v_{2S}/\sqrt{\beta}$. The binding effect reduces electron capture by effectively increasing θ_S to $\epsilon_S\theta_S$. With Nikolaev's OBK cross sections $\sigma_{SS'}^{\text{OBK}}(\theta_S)$ the cross section including the binding effect $\sigma_{SS'}^B$ becomes

$$\sigma_{SS'}^B = \sigma_{SS'}^{\text{OBK}}(\epsilon_S\theta_S). \quad (17)$$

B. Coulomb-deflection effect

The propagation of heavy projectiles ($M_1 \gg 1$) can be treated quantum mechanically or classically with identical results. Specifically the OBK approximation describes the projectile, in the quantum-mechanical version, as a plane wave or, in the semiclassical version, as a classical particle moving along a straight-line trajectory. It neglects the influence of the internuclear repulsion on the motion of the incoming particle.

The Coulomb-deflection effect has been derived for direct ionizations by a classical particle.⁷⁶ In slow collisions, it amounts to a multiplicative factor $\exp(-\pi d q_S)$ where $d = Z_1 Z_2 (M_1^{-1} + M_2^{-1})/v_1^2$ is the half-distance of closest approach in a head-on collision and q_S is the momentum transfer in direct ionization to the continuum state of the target atom with energy $\frac{1}{2}k^2$. This exponential factor can also be obtained by comparing the Coulomb and plane waves at the origin, $R=0$,⁷⁸ since effectively the close collisions are dominating in the slow collision limit.⁷⁹ With the proper normalization procedure for the Coulomb-scattering transition amplitude,^{80,81} one obtains the factor $\exp[-\pi Z_1 Z_2 M(1/K_i - 1/K_f)]$, where $M^{-1} = M_1^{-1} + M_2^{-1}$ and K_i and K_f are initial and final momenta of the particle, respectively. In particular, for electron capture this gives

$$\sigma_{SS'}^C = \exp[-\pi d_{SS'} q_{SS'}(\theta_S)] \sigma_{SS'}^{\text{OBK}}(\theta_S), \quad (18)$$

with

$$d_{SS'} \equiv \frac{Z_1 Z_2 M}{K_i K_f} = d \left/ \left(1 - \frac{M_1 (\frac{1}{2} v_{2S}^2 \theta_S - \frac{1}{2} v_{1S'}^2)}{E_1 M} \right)^{1/2} \right.$$

being the symmetrized version of d and

$$q_{SS'}(\theta_S) \equiv K_i - K_f \approx \frac{\frac{1}{2} v_{2S}^2 \theta_S - \frac{1}{2} v_{1S'}^2}{v_1} + \frac{1}{2} v_1.$$

The use of $d_{SS'}$ instead of d has been argued by Bang and Hansteen⁷⁶ as justified, e.g., by the investigations of the Coulomb excitation of nuclei.^{82,1}

The Coulomb repulsion has been shown to play a crucial role in the OBK calculations of differential cross sections for electron capture.⁸³

We incorporate the binding and Coulomb-deflection effects into the theory for electron capture from S to S' shell as

$$\sigma_{SS'}(v_1 \ll v_{2S}, v_{1S'}) = \exp[-\pi d_{SS'} q_{SS'}(\epsilon_S \theta_S)] \sigma_{SS'}^{\text{OBK}}(\epsilon_S \theta_S), \quad (19)$$

where $v_1 \ll v_{2S}$, $v_{1S'}$ is to stress that this result has been derived for low-velocity ions.

V. COMPARISON WITH EXPERIMENT

To obtain cross sections for electron capture from an inner shell S to all shells S' of fully stripped ions at all velocities, we join⁸⁴ our formulas as derived in the low-, Eq. (19), and high-, Eq. (8), velocity limit and sum⁸⁵ over S' so that

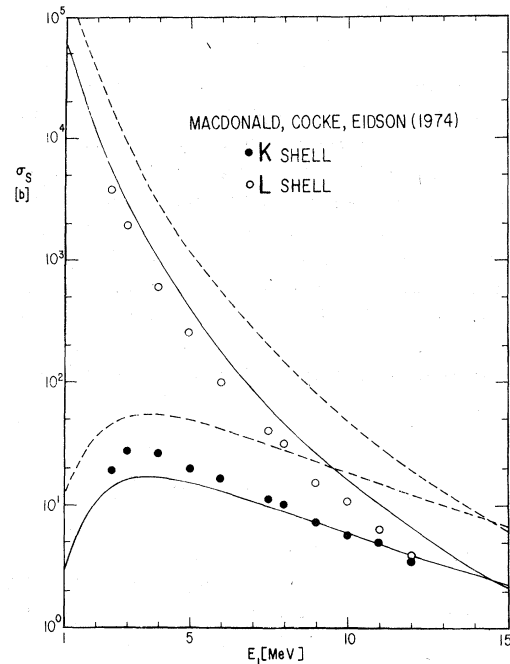


FIG. 2. Electron capture cross sections from K and L shell of argon by protons according to the OBK approximation (Ref. 27) (dashed curves) and the theory as given in Eq. (20) (solid curves). Experimental data are from Ref. 86.

$$\sigma_S = \sum_{S'} \sigma_{SS'} = \sum_{S'} \frac{\sigma_{SS'}(v_1 \gtrsim v_{2S}, v_{1S'}) \sigma_{SS'}(v_1 \ll v_{2S}, v_{1S'})}{\sigma_{SS'}(v_1 \gtrsim v_{2S}, v_{1S'}) + \frac{2}{3} \sigma_{SS'}(v_1 \ll v_{2S}, v_{1S'})} \quad (20)$$

The only direct data for electron capture from inner shells are the cross sections reported by Macdonald, Cocke, and Eidson.⁸⁶ As shown in Fig. 2, the agreement between these data and Eq. (20) is very satisfactory, considering experimental uncertainties in the unraveling of the K-shell cross sections in a coincidence experiment. To test Eq. (20) in slow collisions, we compare it in Fig. 3 with a vast amount of cross sections for total electron capture,⁸⁷⁻⁹⁸ i.e., from all shells, of various target atoms. Agreement is satisfactory except for very slow collisions $v_1 \approx 1$, where our perturbative approach may not be valid. Moreover, in slow collisions, the total electron-capture cross sections are dominated by contributions from outer shells which are poorly described by

the screened hydrogenic wave functions.

To further test Eq. (20) for electron capture from inner shells, we calculated its contribution to ionization of the K shell of argon by fully stripped ions. By adding electron-capture cross sections to direct ionization cross sections,⁹⁹ we improve the agreement with experiments^{2,19,22} as shown in Figs. 4 and 5. In fact, the contribution of electron capture can be as large as that of direct ionization.

Our results may be compared with numerical coupled-state calculations which, however, heretofore have been performed only for relatively simple projectile-target combinations, such as the proton-hydrogen system.¹⁰⁰ Generalizations to systems of arbitrary Z_1 and Z_2 are now beginning to appear.¹⁰¹ For $Z_1/Z_2 \approx \frac{1}{3}$, the present theory for electron capture as well as the theory for direct ionization might be breaking down although more ionization data should be analyzed to affirm such a conclu-

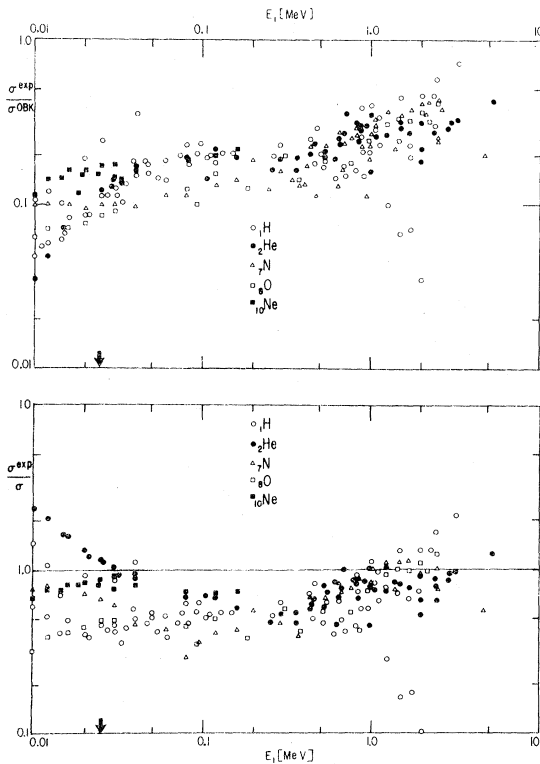


FIG. 3. Ratios of experimental to theoretical cross sections for electron capture from all shells of ^1H , ^2He , ^7N , ^8O , and ^{10}Ne by protons. Experimental data σ^{exp} are from Refs. 87-98; theoretical cross sections are calculated in the OBK approximation (Ref. 27) σ^{OBK} ; and from Eq. (20), σ , in the upper and lower parts of this figure, respectively. The arrow indicates the energy for protons with velocity of one atomic unit.

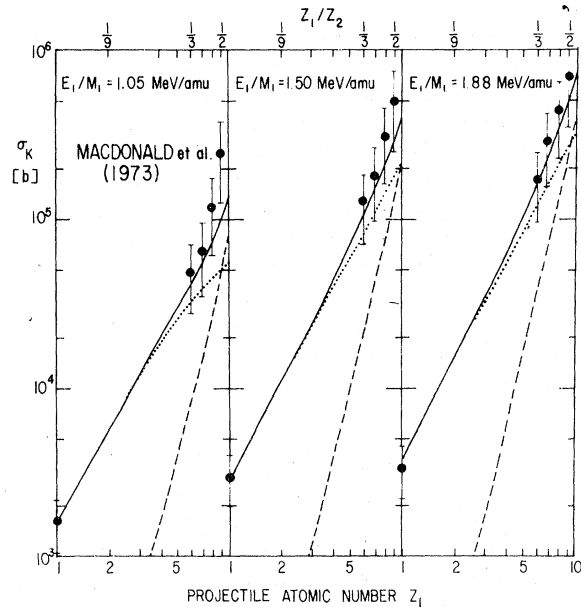


FIG. 4. Cross sections for K-shell ionization of ^{18}Ar by fully stripped ions according to the direct ionization theory (Ref. 99) (dotted curves) and to the electron capture theory as given in Eq. (20) (dashed curves). The solid curves represent the sum of direct ionization and electron capture cross sections. Experimental data are from Ref. 2; error bars include our estimates of uncertainties in fluorescence yields.

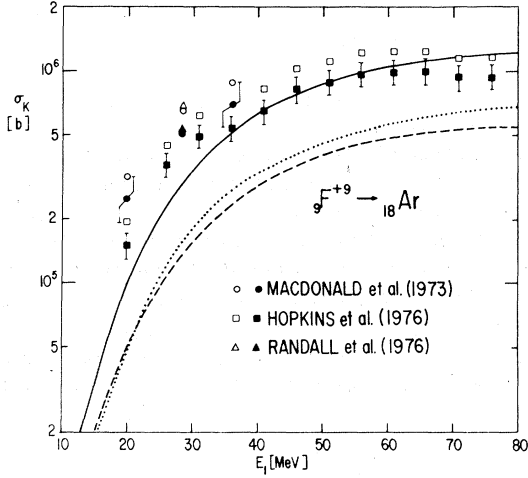


FIG. 5. Cross section for K-shell ionization of ^{18}Ar by fully stripped fluorine according to the direct ionization theory (Ref. 99) (dotted curve) and to the electron capture theory as given in Eq. (20) (dashed curve). The solid curve represents the sum of direct ionization and electron-capture cross sections. Experimental data from Refs. 2, 19, and 22; error bars do not include uncertainties in fluorescence yields. Solid and open symbols show these data when the statistical fluorescence yield ($\omega_K = 0.184$; Ref. 2) and Bhalla's fluorescence yield ($\omega_K = 0.146$; Ref. 19) are used, respectively.

sion. Experiments for which electron capture is not negligible, i.e., experiments with the systems for which Z_1/Z_2 is not very small, ought to be performed with low- and high-velocity ions to test the theory. Direct measurements of electron capture from inner shells, such as those obtained from coincidence experiments,⁸⁶ are needed.

In summary, we have developed a theory for electron capture from inner shells by fully stripped ions, and found it to be in satisfactory agreement with experiment. In fact, electron capture becomes an important channel of inner-shell Coulomb ionization as Z_1/Z_2 increases.

ACKNOWLEDGMENTS

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APPENDIX A: IMPACT-PARAMETER-DEPENDENT FUNCTIONS FOR ELECTRON CAPTURE

In a semiclassical approximation, the differential cross section with regard to impact parameter p can be given in terms of the reduced variable

$$x_{SS'} \equiv p\sqrt{\beta} = (q_{SS'}^2 + v_{1S'}^2)^{1/2} p \text{ as}$$

$$d\sigma_{SS'}(x_{SS'}) = \sigma_{SS'} 2\pi P_{SS'}(x_{SS'}) x_{SS'} dx_{SS'}, \quad (\text{A1})$$

where $P_{SS'}$ is an impact-parameter-dependent function which is related to the transition amplitude $a_{SS'}$ and normalized such that

$$2\pi \int_0^\infty P_{SS'}(x) x dx = 1.$$

In terms of the weight function $W_{SS'}$,

$$\begin{aligned} W_{SS'}(x_{SS'}) &\equiv \sum_{s' \in s'} |a_{sS'}(x_{SS'})|^2 \\ &\times \left(\int_0^\infty \sum_{s' \in s'} |a_{sS'}(x_{SS'})|^2 x_{SS'} dx_{SS'} \right)^{-1}, \end{aligned} \quad (\text{A2})$$

$P_{SS'} = W_{SS'}/2\pi$. In the following we consider transition amplitudes obtained in the OBK approximation.

The OBK cross section had been derived by Brinkman and Kramers²⁶ in the high projectile-velocity limit of the semiclassical approximation for electron transfer between the ground states of hydrogen and proton. Their a_{KK}^{OBK} can be easily generalized to $a_{SS'}^{\text{OBK}}$ for the collision systems under our consideration by substituting β for $1 + (\frac{1}{2}v_1)^2$. However, we need to know $a_{SS'}^{\text{OBK}}$ in the slow-collision limit for the derivation of the binding effect in Sec. IV.

Bates and McCarroll^{30,102} demonstrated that the factor $\exp(-iv_1 z)$ has to be introduced into the transition amplitude to account for the translational motion of the electron¹⁰³ and to prove the equivalence of the quantum-mechanical and semiclassical treatments for electron capture in slow collisions. With the z axis denoting the straight-line trajectory of the projectile [see, e.g., Eq. (A 4.3.16) of Ref. 35], one obtains¹⁰⁴

$$\begin{aligned} a_{SS'}^{\text{OBK}} &= \frac{1}{(2\pi)^2 v_1} \\ &\times \int d^3k' f_s(\vec{k}) g_{S'}^*(\vec{k}') \delta(k'_z - q_{SS'}) e^{i\vec{k}' \cdot \vec{z}}, \end{aligned} \quad (\text{A3})$$

where

$$f_s(\vec{k}) \equiv \int \psi_s(\vec{r}) e^{i\vec{k} \cdot \vec{r}} d^3r, \quad (\text{A4})$$

$$g_{S'}(\vec{k}') \equiv \int \psi_{S'}(\vec{r}) \frac{Z_1}{r} e^{i\vec{k}' \cdot \vec{r}} d^3r,$$

and [see e.g., Eq. (8.2.10) of Ref. 35]

$$k^2 + v_{2S}^2 \theta_S = k'^2 + v_{1S'}^2. \quad (\text{A5})$$

In particular, for electron capture from a

screened hydrogenic K shell to a hydrogenic K' shell one gets

$$f_K(\vec{k}) = \frac{8\pi^{1/2}v_{2K}^{5/2}}{(k^2 + v_{2K}^2)^2} \quad (A6)$$

and

$$g_{K'}(\vec{k}') = \frac{4\pi^{1/2}v_{1K'}^{5/2}}{k'^2 + v_{1K'}^2},$$

so that

$$\begin{aligned} a_{KK'}^{\text{OBK}} &= \frac{8(v_{1K'}v_{2K})^{5/2}}{\pi v_1} \int_{-\infty}^{\infty} dk_x e^{ipk_x} \\ &\times \int_{-\infty}^{\infty} \frac{dk_y}{[k_x^2 + k_y^2 + \beta + (1 - \theta_K)v_{2K}^2](k_x^2 + k_y^2 + \beta)} \\ &\propto K_0[x_{KK'}(1-c)^{1/2}] - K_0(x_{KK'}) - \frac{1}{2}c x_{KK'} K_1(x_{KK'}), \end{aligned} \quad (A7)$$

where $c \equiv (1 - \theta_K)v_{2K}^2 / [\beta + (1 - \theta_K)v_{2K}^2]$ and K_0 and K_1 are the modified Bessel functions of zeroth and first order, respectively. We obtain¹⁰⁵

$W_{KK'}(x_{KK'})$

$$= \frac{\{K_0[x_{KK'}(1-c)^{1/2}] - K_0(x_{KK'}) - \frac{1}{2}c x_{KK'} K_1(x_{KK'})\}^2}{\frac{3}{2} + \frac{1}{2}c + \frac{1}{8}c^2 + \frac{1}{2}(1-c)^{-1} + (2/c)\ln(1-c)} \quad (A8)$$

In the $c \rightarrow 0$ limit, Eq. (A8) reduces to

$$W_{KK'}(x_{KK'}; c \rightarrow 0) = \frac{5}{32} x_{KK'}^4 K_2^2(x_{KK'}), \quad (A9)$$

which is identical with the W_K function for direct ionization of the K shell in the slow-collision limit.⁷¹ With few exceptions, c is in the range 0.001 to $\frac{2}{3}$. For such c , Eq. (A8) gives the same

numerical values as Eq. (A9) to within at most 30% over the range $0 \leq x_{KK'} \leq 2.5$ from which significant contributions may come to the integral in Eq. (12). In fact, with typical values of $c < \frac{1}{3}$, Eq. (12) gives the same results to within 5% for $W_{KK'}$ of Eqs. (A8) and (A9) (see Fig. 1).

Following the above procedure, it can be shown, after somewhat lengthy calculations, that $W_{SS'}$ for electron capture from the S subshells and W_S for direct ionization are identical functions when derived in the slow-collision limit. An analytical approximation to $W_K = W_{L_1}$, Eqs. (A9) and (16) of Ref. 72, is given by Eq. (A3) of Ref. 72. The second equation in Eq. (16) of this reference is in error and should be replaced by

$$W_{L_2, L_3}(x) = \frac{1}{192} x^9 [K_3^2(x) + K_2^2(x)], \quad (A10)$$

which can be approximated with errors less than 1% by

$$W_{L_2, L_3}(x) = \frac{1}{3}(1 + 2x + 1.8x^2 + x^3 + 0.3x^4 + \frac{1}{64}\pi x^5)e^{-2x}. \quad (A11)$$

APPENDIX B: SAMPLE CALCULATION OF CROSS SECTION FOR ELECTRON CAPTURE

We illustrate the scheme of calculation for electron capture from the K shell of argon ($Z_2 = 18$, $M_2 = 40 \times 1823$) by a 12.6-MeV ion of carbon ($Z_1 = 6$, $M_1 = 12 \times 1823$). The orbital velocities of the electron before and after the collision are $v_{2K} = 18 - 0.3 = 17.7$ and $v_{1S'} = 6/n_1$, respectively; while the velocity of the ion is $v_1 = 6.50$. With 3203 eV for the observed binding energy of the argon K shell,¹⁰⁶ one obtains $\theta_K = 3203 / (\frac{1}{2} \times 6.5 \times 6.5 \times 27.2) = 0.752$. Since $(v_{2K}^2 \theta_K - v_{1S'}^2) / M_1 v_1^2 \ll 1$, it is sufficient to calculate $d_{KS'}$ and $q_{KS'}(\theta_K)$ as

TABLE I. Electron-capture cross sections in barns and quantities required for their computation. The numerical values pertain to the sample calculation delineated in Appendix B for electron capture from the K -shell of argon by 12.6 MeV fully stripped ions of $^{12}_6\text{C}$.

Quantity	S'=K ($n_1=1$)	S'=L ($n_1=2$)	S'=M ($n_1=3$)	S'=N ($n_1=4$)	Ref. or Eq.
$\sigma_{KS'}^{\text{OBK}}(\theta_K=0.752)$	1.9×10^5	1.3×10^4	3.5×10^3	1.4×10^3	Ref. 27
$q_{KS'}(\theta_K=0.752)$	18.6	20.7	21.1	21.2	Eq. (B2)
$v_{2K} \sqrt{\beta}$	0.908	0.847	0.835	0.831	Eq. (B3)
$g_K(v_{2K} \sqrt{\beta})$	0.604	0.625	0.630	0.631	Eq. (14)
$\epsilon_K \theta_K$	1.54	1.56	1.57	1.57	Eq. (13)
$q_{KS'}(\epsilon_K \theta_K)$	28.4	30.8	31.5	31.5	Eq. (B2)
$\exp[-\pi d_{KS'} q_{KS'}(\epsilon_K \theta_K)]$	0.987	0.986	0.985	0.985	Eq. (19)
$\sigma_{KS'}(v_1 < v_{2K}, v_{1S'})$	8.2×10^3	5.3×10^2	1.3×10^2	5.5×10^1	Eq. (19) and Ref. 27
$\sigma_{KS'}$	7.6×10^3	4.9×10^2	1.2×10^2	5.1×10^1	Eqs. (20), (19), (8), and Ref. 27

$$d_{K_S'} \approx d = \frac{Z_1 Z_2}{M v_1^2} = \frac{6 \times 18 \times (12 + 40)}{12 \times 40 \times 1823 \times (6.50)^2} = 0.0015 \quad (\text{B1})$$

and

$$q_{K_S'}(\theta_K) = \frac{\frac{1}{2}(v_{2K}^2 \theta_K - v_{1S'}^2)}{v_1} + \frac{1}{2}v_1 \\ = \frac{117.8 - 18/n_1^2}{6.50} + 3.25 = 21.4 - \frac{2.8}{n_1^2}. \quad (\text{B2})$$

The numerical values of $q_{K_S'}(\theta_K)$,

$$\frac{v_{2K}}{\sqrt{\beta}} = \frac{17.7}{[(21.4 - 2.8/n_1^2)^2 + 36/n_1^2]^{1/2}}, \quad (\text{B3})$$

$g_K(v_{2K}/\sqrt{\beta})$, $\epsilon_K \theta_K$, $q_{K_S'}(\epsilon_K \theta_K)$, and $\exp[-\pi d_{K_S'}$

$\times q_{K_S'}(\epsilon_K \theta_K)]$ are listed in Table I for $n_1 = 1, 2, 3$, and 4. The cross sections $\sigma_{K_S'}^{\text{OBK}}(\theta_K)$, $\sigma_{K_S'}(v_1 \ll v_{2K}, v_{1S'})$, and $\sigma_{K_S'}$ are also displayed in this Table. On summing over all four S' shells in the first and last line of Table I, one gets $\sigma_K^{\text{OBK}}(\theta_K) = 2.1 \times 10^5$ b, and $\sigma_K = 8.3 \times 10^3$ b in the OBK approximation and present theory, Eq. (20), respectively. By adding these electron capture cross sections to the direct K-shell-ionization cross section, 3.1×10^4 b,⁹⁹ we obtain correspondingly 2.4×10^5 b and 3.9×10^4 b for K-shell ionization by the 12.6-MeV carbon ions. The experimental value² deduced from the x-ray production cross section with the statistical fluorescence yield ($\omega_K = 0.162$) is 4.9×10^4 b.

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