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TRANSITION PROBABILITIES AND MULTIPLE IONIZATIONS OF IONS
BY HIGH ENERGY ELECTRON IMPACT

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ABSTRACT

The single-particle model for atoms and ions is used to calculate the transition probabilities to bound and continuum electronic states. The projection operators in the semi-classical approximation derived previously are applied to treat the large numbers of final states involved. Ionization cross sections of atoms and ions by high-energy electron impact are then estimated, which result both from direct transition to the continuum and from inelastic scattering followed by the Auger emission.

I. INTRODUCTION

Electron impact provides a possible mechanism for production of highly ionized beams to be used for injection into heavy ion accelerators. With most of the periodic table and as many as twenty to thirty steps of ionization considered of interest, it is evident that several thousand ionization cross sections may be required to estimate ionization rates. It is also evident that great accuracy is not feasible in the calculation of so many cross sections. The purpose of this paper is to obtain a reasonable estimate in parametrized form for the many required cross sections.

We shall assume the bombarding electrons to have energies large compared with the relevant electronic ionization potentials. Two mechanisms for ionization will be considered; (a) direct transitions to continuum states; (b) excitations of inner shell electrons to excited states followed by Auger emission. Several studies of the fluorescence yield\(^1-3\) indicate that process (b) is no less important than (a) for producing ionization.

To obtain a quantitative estimate of the contribution from the processes (a) and (b), it is desirable first to evaluate the transition probabilities of both inner- and outer-shell electrons to various allowed excited states, including the continuum. For the target atoms and ions, we choose a simple single-particle model. Based on the extensive studies carried out earlier using the Hartree-Fock\(^4\) and Fermi-Thomas models,\(^5\) Green et al.\(^6\) have derived an even simpler model for complex atoms, with analytic potentials of the Coulombic plus Wood-Saxon type. Although rather crude in the prediction of term values, this model is probably sufficient for our present purpose. The form
of potential we have adopted contains essentially one adjustable parameter \( d \) for each core charge \( Z_C \).

The transition probabilities to a group of excited states and the continuum may be conveniently evaluated using the projection operators derived earlier\(^7\) in the semi-classical approximation. Since the model potential we have chosen is local and in a single-particle form, very little modification is necessary; we have used the simple form \( \psi_{BO}^i \) in the notation of Ref. 7.

In Sec. II, we define the model potential for the target ions. Since we present the result of our calculations at only several typical values of \( Z_C \) and the degree of ionization \( Z_I \), the intermediate steps involved in the energy eigenvalue calculations and scaling should be helpful in obtaining results at other values of \( Z_C \) and \( Z_I \). We give a brief discussion of this in Appendix A. The transition probabilities with dipole coupling are defined in terms of the semi-classical projection operators, and the complete set of transitions allowed by the selection rules and exclusion principle is studied.

The result of Sec. II is then used in Sec. III to estimate the ionization cross sections of ions and atoms by high-energy electron impact. Contributions from the different competing processes mentioned above are evaluated. With the various simplifying approximations which are expected to be valid for high-energy collisions, the transition probabilities evaluated in Sec. II can be directly related to the ionization cross sections.

II. THE SINGLE-PARTICLE MODEL AND TRANSITION PROBABILITIES

For simplicity, we adopt the single-particle potential for atoms and ions obtained by Green et al.,\(^6\) which was derived by fitting the HF and HFS solutions. Its form is

\[
V(r) = \frac{1}{\nu} \left[ (Z_C - Z_I - 1) Y(r) - Z_C \right],
\]

(2.1)

where

\[
Y(r) = 1 - \bar{u}(r),
\]

(2.2)

where

\[
\bar{u}(r) = [H(e^r/d - 1) + 1]^{-1}
\]

and

\[
H = \alpha(Z_C - Z_I - 1)^\nu d
\]

\[
\nu = 0.4
\]

\[
\alpha = 1.00
\]

\[
m = \pi = e^2 = 1\]

for all \( Z_C \) and \( Z_I \).

Thus, the only parameter which is varied as a function of \( Z_C \) is \( d \), which is assigned the values\(^6\) given in Table I. (We take Green's values.)
The result of the calculation of the single-particle energies \( E_{n\ell} \) is summarized in Tables II-IV for the value \( Z_c = 10, 20, \ldots, 80 \). For each \( Z_c \), all values of \( Z_I \) which correspond to the filled subshells are considered.

As \( V(r) \) of (2.1) is Coulombic for large values of \( r \), we expect to have an infinite number of bound states near each ionization threshold. Therefore, the excitation probabilities to these discrete and also to continuum states may be evaluated most conveniently using projection operators. We have shown previously that the projection onto all the bound states generated by the potential \( V(r) \) may be given in a semi-classical approximation by

\[
\lambda_+^{±}(r, r') = \frac{1}{\pi r} \sin(P_u),
\]

where

\[
P(v) = \left[ -2V(r) - \frac{L_+^2}{v^2} \right]^{1/2}
\]

and

\[
\mu = r - r', \quad v = (r + r')/2
\]

\[
L_+^2 = (\ell_+ + \frac{1}{2})^2.
\]

In (2.5), \( \ell_+ = \ell + 1 \) are the angular momenta of the excited states reached by the dipole coupling from the initial state with the angular momentum \( \ell \).

For a more general case in which the projection onto states which lie between \( E_a \) and \( E_b \) is desired, we have

\[
\lambda_+^{±}(r, r') = \frac{1}{\pi r} \sin(P_u) - \sin(P_v)
\]

where

\[
P_a(v) = \left[ 2E_a - 2V(v) - L_{±}^2 v^{-1} \right]^{1/2}
\]

\[
P_b(v) = \left[ 2E_b - 2V(v) - L_{±}^2 v^{-1} \right]^{1/2}
\]

\[
E_a < E_b < 0.
\]

Note that, in the rescaled units of Appendix A,

\[
P_a(\overline{v}) = \left[ \frac{E_a}{4E_{n\ell}} - \frac{V(\overline{v})}{(E_{n\ell})^2} - \frac{L_{±}^2}{\overline{v}^2} \right]^{1/2}
\]

with

\[
\overline{v} = (s + s')/2, \quad s = 2(E_{n\ell})^{1/2} r, \quad (E_{n\ell} > 0).
\]

In particular, we choose in the following \( E_a = E_b \), \( E_b = 0 \), which gives \( \lambda_+^{±} \rightarrow \lambda_{ab}^{±} \) for the projections onto states which lie between \( E_D \) and the ionization threshold.

For dipole coupling, the integrals of interest here are then given by

\[
\langle n\ell | s | n\ell \rangle
\]

\[
\langle n\ell | s^+ | n\ell \rangle
\]
The values for $E_b$ are chosen such that the transitions are only to the unoccupied levels of given $\ell = \ell \pm 1$, in accordance with the exclusion principle. Therefore, $M_D$ corresponds to the correct transition probability to all the unoccupied bound states of the ion with $Z_C$ and $Z_I$, while $M_B$ includes transitions to all bound levels, some of which are forbidden by the exclusion principle. Throughout the calculation, we have taken $E_D$ to be the $E_{n\ell}$ corresponding to the last filled subshell energies. Table V contains a sample for $Z_C = 20$.

The accuracy of the projection operators $\Lambda_B$ and $\Lambda_D$ is partly reflected in the integral

$$S_{n\ell} = \langle n\ell | \Lambda_B^{\ell} | n\ell \rangle,$$

which should be unity if $\Lambda_B^{\ell}$ were exact and the state $| n\ell \rangle$ is contained in $\Lambda_B^{\ell}$. This value is also given in Table V. We refer the readers to Ref. 7 where the accuracy of $\Lambda_B^{\ell}$ was studied in detail for several cases where exact results are available for comparison. Except when $M_B$ or $M_C$ are very small compared with $M_A$, we expect our result to be fairly reliable.

Relativistic corrections are expected to be significant for K-shell electrons when $Z_C \geq 50$. Because these inner electrons contribute little to the ionization processes when $Z_C > 40$, [see Fig. (2)], we have ignored relativistic corrections to the atomic structure. The projectile electrons will be treated relativistically, however, in our final results.

Finally, it is of interest to compare the transition probabilities to the continuum calculated here with those for hydrogenic atom given in Ref. 8. For this purpose, we write

$$\tilde{\gamma}_{n\ell} = \left[ \frac{(\ell + 1) M_C^{n\ell+} + \ell M_C^{n\ell-}}{2\ell + 1} \right] \left( E_{n\ell}/\beta \right),$$

where the factor $1/3$ is the average of the orientation of the dipole operators in (2.8) - (2.10). Table VI contains the result for $Z_C = 10$ and $Z_C = 60$, with $Z_I = 0$. Figure 1 also contains the result for $Z_C = 30$. 
III. TOTAL IONIZATION CROSS SECTIONS

We consider the collision of a fast electron of momentum \( k_0 \) (energy \( \epsilon_0 = k_0^2 / 2m \) large compared with single orbital ionization energies) with an ion characterized by the charge parameters \((Z_0, Z_1)\).

The collision leads to a single orbital transition \( \alpha \rightarrow \beta \), where \( \alpha = n, l, \ldots \). The final momentum of the impacting electron is \( k_\beta \), where

\[
\epsilon_\beta = \frac{k_\beta^2}{2m} = \epsilon_0 - \Delta_\alpha \beta, \quad (3.1)
\]

Neglecting exchange terms involving the impacting electron, we may write the differential cross section in the form given by Kott and Kassey

\[
I_\alpha^{(\beta)}(\Omega) = \left( \frac{m}{2\pi} \right)^2 \frac{k_\beta}{k_0} Z_\alpha \int \int d^3r \ d^3\mathbf{r}_0 \ \phi^*_\beta(r) \phi_\alpha(r) e^{i\mathbf{q} \cdot \mathbf{r}} \left| \mathbf{v}_s \right|^2, \quad (3.2)
\]

where the \( \phi \)'s are single electron orbital states,

\[
\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_\beta = q \mathbf{\hat{n}}, \quad (3.3)
\]

\( \mathbf{\hat{n}} \) is the scattering angle, and

\[
\mathbf{v}_s = \frac{e^2}{|\mathbf{r}_0 - \mathbf{r}|}, \quad (3.4)
\]

We take \( Z_\alpha \) to be the number of electrons in the shell \( \alpha = (n, l, \ldots) \).

For high energy impacts, we may use the dipole approximation

\[
\int d^3r_0 \ e^{i\mathbf{q} \cdot \mathbf{r}_0} \mathbf{v}_s = \frac{4\pi e^2}{q^2} e^{i\mathbf{q} \cdot \mathbf{r}} \approx \frac{4\pi e^2}{q^2} (1 + i\mathbf{q} \cdot \mathbf{\hat{n}}), \quad (3.5)
\]

Thus,

\[
I_\alpha^{(\beta)}(q) = 8\pi \left( \frac{k_\beta}{k_0q^2} \right)^2 Z_\alpha \ K_\alpha^{(\beta)}, \quad (3.6)
\]

where

\[
K_\alpha^{(\beta)} = \left| \int d^3r \ \phi^*_\beta(r) \phi_\alpha(r) \mathbf{\hat{n}} \right|^2 / (a_0)^2. \quad (3.7)
\]

Now,

\[
k_0 k_\beta \sin \Omega d\Omega = q dq \approx k_0^2 \sin \Omega d\Omega, \quad (3.8)
\]

so we may introduce

\[
J_\alpha^{(\beta)}(q) dq = 2\pi I_\alpha^{(\beta)}(q) k_0 k_\beta \sin \Omega d\Omega / q, \quad (3.9)
\]

or the total cross section

\[
\sigma_\alpha^{(\beta)}(k_\alpha) = \int_{q_{\min}}^{q_{\max}} J_\alpha^{(\beta)}(q) dq \approx \frac{4\pi Z_\alpha}{k_0^2} k_\alpha \ln \left( \frac{4 \epsilon_0}{\Delta_\alpha \beta} \right). \quad (3.10)
\]

Here, we have used high energy, nonrelativistic kinematics to determine the limits on \( q \) as

\[
q_{\min} \approx \frac{m \Delta_\alpha \beta}{k_\alpha}, \quad (3.11)
\]

\[
q_{\max} \approx \left( 2 m \epsilon_0 \right)^{1/2}.
\]
We consider first the direct ionization to continuum states. When the expression (3.9) for $\sigma_{\alpha\beta}$ is summed over all available final states, we have

$$
\sigma_{\alpha}(k_{\alpha}) = \sum_{\beta} \sigma_{\alpha\beta} \approx \sum_{\beta} \frac{4\pi Z_{\alpha}^{2}}{k_{\alpha}^{2}} M_{\alpha\beta} C \ln \left( \frac{4\pi}{\hbar e_{\alpha}^{2} C} \right) 
$$

(3.12)

where

$$
M_{\alpha\beta} = \sum_{C} M_{\alpha\beta} C, \quad \alpha = (n, l) 
$$

(3.13)

$\Delta_{\alpha}^{C}$ = the average excitation energy defined by (3.12).

Since both $e_{1}^{+}$ and $e_{1}^{-}$ are involved in our case, we replace $M_{\alpha\beta} C$ in (3.12) by its average

$$
\overline{M}_{\alpha\beta}^{n} = \frac{1}{3(2l + 1)} [(l + 1) M_{\alpha\beta}^{n+} + l M_{\alpha\beta}^{n-}] = \overline{M}_{\alpha\beta}^{0} 
$$

(3.14)

and set

$$
Z_{\alpha} \equiv Z_{n_{l}} = 2(2l + 1), \text{ for each closed subshell.} 
$$

(3.15)

Thus, combining (3.12) - (3.15), we finally have

$$
\sigma_{\alpha}(k_{\alpha}) = (\pi a_{0}^{2}) \frac{4\pi Z_{\alpha}^{2}}{(k_{\alpha} a_{0})^{2}} \ln \left( \frac{4\pi}{\hbar e_{\alpha}^{2} C} \right) \overline{M}_{\alpha\beta}^{0}, \text{ (NR)} 
$$

(3.16)

and thus

$$
\sigma^{C}(z_{C}, z_{T}, E) = \sum_{\alpha} \sigma_{\alpha} C. 
$$

(3.17)

As discussed earlier, the ionization of the target ions is also possible through the excitation of an inner-shell electron followed by an Auger transition. This is then related to the transition matrix elements $M_{D}^{n_{l}}$ to all the allowed bound state levels and also to the fluorescence yield. If we denote by $W_{\alpha}$ the probability that an Auger transition will follow excitation from the orbital state $\alpha$, the cross section for ionization following collisional excitation is

$$
\sigma_{\alpha}(k_{\alpha}) = (\pi a_{0}^{2}) \frac{4\pi Z_{\alpha}^{2}}{(k_{\alpha} a_{0})^{2}} \ln \left( \frac{4\pi}{\hbar e_{\alpha}^{2} C} \right) \overline{M}_{D}^{0} W_{\alpha}, \text{ (NR)} 
$$

(3.18)

which follows from the argument similar to that was used to obtain (3.16), and thus

$$
\sigma^{A}(Z_{C}, Z_{T}, E) = \sum_{\alpha} \sigma_{\alpha} A. 
$$

(3.19)

In (3.18), $W_{\alpha}$ are given by the fluorescence yield $Y_{\alpha}$ as $W_{\alpha} = 1 - Y_{\alpha}$, and the actual values used in our calculation are given in Fig. 2, with $W_{\alpha} = 1$ for $n \geq 3$; $\Delta_{\alpha}^{B}$ is the average excitation energy of the $g$th subshell, and

$$
\overline{M}_{D}^{0} = \frac{1}{3(2l + 1)} [(l + 1) M_{D}^{n_{l}+} + l M_{D}^{n_{l}^-}] \cdot 
$$

(3.20)
The total ionization cross section is finally given by

\[ \sigma^T(Z_C, Z_I, E) = \sum_\alpha (\sigma_\alpha^C + \sigma_\alpha^A) \]  

(3.21)

for each set of parameters \( Z_C, Z_I, \) and \( E. \)

In actual calculation, we simply used

\[ \Delta_\alpha^C = \Delta_\alpha^B = E_I \]  

(3.22)

where \( E_I \) is the ionization potential for the electron in the highest filled subshell. Since the cross sections depend on \( \Delta \) only logarithmically, the choice (3.22) is not expected to affect the result drastically. An improved treatment of the log factor is possible, however, and this is outlined in Appendix B, where a procedure to estimate the average excitation energy is presented.

When the incident electron is relativistic, we have to modify (3.16) and (3.18) slightly as

\[ \log \left( \frac{\hbar e_\alpha}{\Delta_\alpha^C} \right) \rightarrow \left[ \log \left( \frac{\hbar e_\alpha^\gamma}{\Delta_\alpha^C} \right) - \beta^2 \right] \]  

(3.23)

and

\[ k a_0^a \rightarrow \beta/\alpha_0 \]  

(3.24)

where

\[ \alpha_0 = \frac{e^2}{\hbar c} = \frac{1}{137} \]

\[ \gamma = (1 - \beta^2)^{-\frac{1}{2}}, \quad \beta = v/c. \]

Thus, we have explicitly, at high energies with relativistic electron beams and with \( E = \gamma mc^2 \),

\[ \sigma_\alpha^C = (\pi a_0^2) \frac{\hbar e_0^2}{\beta^2} \left[ \log \left( \frac{2\beta^2 E}{\Delta_\alpha^C} \right) - \beta^2 \right] Z_\alpha \bar{w}_C^\alpha, (ER) \]  

(3.25)

\[ \sigma_\alpha^A = (\pi a_0^2) \frac{\hbar e_0^2}{\beta^2} \left[ \log \left( \frac{2\beta^2 E}{\Delta_\alpha^B} \right) - \beta^2 \right] Z_\alpha \bar{w}_D^\alpha \bar{w}_\alpha, (ER). \]  

(3.26)

In Table VII, both nonrelativistic forms (3.16), (3.18), and the extreme relativistic forms (3.25), (3.26) of cross sections are used to calculate the total ionizations. The result at \( E = 1 \text{ KeV} \) and at 10 KeV seems to agree reasonably well with the earlier calculations and also with the experimental value. We note that the contribution of \( \sigma^A \) is not negligible.

Individual values of \( \sigma^C \) and \( \sigma^A \) for various \( Z_C \) and \( E = Z_C - Z_I \) are presented in Fig. 3. For given \( Z, \sigma^C \) seems to dominate at small \( Z_C \), but this trend is reversed for large \( Z_C \), with \( \sigma^A \) dominating at high \( Z_C \). The total ionization cross section \( \sigma^T \) is given in Fig. 4 for an electron energy of 20 KeV. The cross section at other energies may be scaled from Fig. 4 and Eqs. (3.10), (3.18), (3.25), and (3.26).
IV. DISCUSSION

The ionization cross sections that we have obtained in Section III are based on a rather crude model for the electron orbital states. The comparisons in Tables VI and VII with the corresponding exact calculations given in Ref. 8 (for hydrogen, however, so that direct comparison is not possible) and with some experimental cross sections provide an indication of the accuracy of our cross sections. We have made several of the 'standard' high energy approximations and these of course limit the energy range over which our expressions can be used.

The previous estimates\(^3\) of \(\sigma^I\) do not include the contribution of \(\sigma^A\), which requires both \(\bar{n}_D\) and \(\bar{n}_A\). Since \(\sigma^A\) seems to dominate the ionization cross sections at high \(Z\), any agreement existed previously between the theoretical calculations and experiments could be fortuitous.

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APPENDIX A

The calculation of the eigenvalues and eigenfunctions with the local potential \( V(r) \) given in Sec. II is well known, but we briefly describe the procedure used in our calculation so that results at other values of \( Z_C \) and \( Z_I \) than those presented here could be readily reproduced.

The single-particle energies and wave functions are calculated in the usual way by solving the radial equation

\[
\left[ -\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + 2V(r) + E_n\ell \right] R_n\ell(r) = 0 , \quad (A.1)
\]

where \( E_n\ell \) is given in Rydberg units. Since a large variation in \( Z_C \) and \( E_n\ell \) is involved, we rescale the variable \( r \) such that (A.1) becomes

\[
\left[ -\frac{d^2}{ds^2} + \frac{\ell(\ell + 1)}{2(E_n\ell)^2 s^2} + \frac{\ell + \frac{1}{2} - \frac{1}{4}}{s^2} \right] R_n\ell(s) = 0 , \quad (A.2)
\]

with

\[
s = 2(E_n\ell)^{\frac{1}{2}} r , \quad (E_n\ell > 0)
\]

\[
V(s) = V\left[r \rightarrow s, \quad d \rightarrow d' = 2(E_n\ell)^{\frac{1}{2}} d\right] .
\]

The solutions obtained by integrating (A.2) in from the large values of \( s \) and out from \( s = 0 \) are matched at \( s = s_0 \), \( s_0 = 20 h \) with \( h = 0.2 \) in the above unit.

The starting values for the integrations are calculated as follows:

\[
\begin{align*}
(a) \quad s = 0 \quad \text{region:} \\
& \text{Using the expansion of the regular Whittaker function,}^{10} \\
R_n\ell(s) = W_{\frac{m}{2} - \frac{1}{2}}(s) = s^{\frac{1}{4}m} e^{-\frac{1}{2}s} \left\{ 1 + \frac{\frac{3}{2} + m - k}{1l(2m + 1)} s \right. \\
& \left. + \frac{\frac{3}{2} + m - k(\frac{3}{2} + m - k)}{2l(2m + 1)(2m + 2)} s^2 + \ldots \right\} , \quad (A.3)
\end{align*}
\]

where

\[
k = \frac{Z_C}{(E_n\ell)^{\frac{1}{2}}}
\]

\[
m = \frac{1}{2} .
\]

That is, the dominant part of \( V(r) \) near \( r = 0 \) is taken to be purely Coulombic with the charge \( Z_C \). The correction to the wave function coming from the non-Coulombic part of \( V(s) \) is then included by integrating out with the finer mesh size \( h' = 0.1h \). In this way, the starting values of \( R_n\ell \) and \( R_n'\ell \) at \( s = h \) for further integration outward with \( \Delta s = h \) are generated.

\[
(b) \quad s \text{ large:}
\]

Since the core charge \( Z_C \) is in general screened by the \( (Z_C - Z_I - 1) \) electrons, we have to modify the value of \( k \) in the region of large \( s \), as

\[
k \rightarrow k = \frac{(Z_I + 1)}{(E_n\ell)^{\frac{1}{2}}}
\]

\[
m = \frac{1}{2} .
\]

Thus, we have\(^{10}\)
\[ R_{n\ell} = W_{km}(s) = e^{\frac{s}{2}} s^k \left\{ 1 + \frac{m^2 - (s - \frac{1}{2})^2}{1! s} \right\} \]

\[ + \left[ \frac{m^2 - (s - \frac{1}{2})^2}{1! s^2} \left[ \frac{m^2 - (s - \frac{3}{2})^2}{2! s^2} + \ldots \right] \right] \]  

**(A.4)**

Typically, the starting values are evaluated at \( s = 27 \) in the rescaled atomic units.

(c) The matching of the logarithmic derivatives is made at \( s = s_0 = 20h, \ h = 0.2 \), except when they are very small in this region.

The value of \( E_{n\ell}^{(t)} \) guessed initially is corrected by the formula

\[ E_{n\ell} = E_{n\ell}^{(t)} + \Delta_{n\ell} \]

where

\[ \Delta_{n\ell} = \left[ \int_0^{s_0} u_t^2 ds / (u_t^2|_{s=s_0}) + \int_{s_0}^{\infty} v_t^2 ds / (v_t^2|_{s=s_0}) \right] \]

\[ \cdot [v_t/v_t - u_t/u_t]^{-1} \]  

**(A.5)**

In \((A.5)\), \( u_t \) and \( v_t \) are the functions obtained by integrating out and in, respectively. With a reasonable initial guess on \( E_{n\ell}^{(t)} \), the procedure converged within five iterations to an accuracy of one part in \( 10^4 \). Note that the variable \( r \) is rescaled as \( E_{n\ell} \) is changed.

In view of the crudeness of the model used, the eigenvalues \( E_{n\ell} \) are not expected to be very accurate, especially for the higher excited states. In fact, the variations among the values obtained with different models are substantial. Therefore, \( R_{n\ell} \) and \( E_{n\ell} \) are calculated here only to the accuracy which is sufficient to give a rough estimate of the excited states involved.
APPENDIX B

The average excitation energies $\Delta^B_\alpha$ and $\Delta^C_\alpha$ introduced in Sec. III may be estimated more accurately if we write, by definition,

$$M^\alpha_B \ln \left( \frac{h_\alpha^B}{\Delta^B_\alpha} \right) = \sum_\beta (\alpha| r^B_\alpha - r^\beta_\alpha | \beta)^2 \ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right), \quad (B.1)$$

and similarly for $\Delta^C_\alpha$ where $M^\alpha_C$ is given by (3.13). The range of the $\beta$-sum is such that

$$0 < E^B_\alpha - E^D_\alpha < \Delta^B_\alpha < E^D_\alpha$$

$$E^B_\alpha < \Delta^C_\alpha < \infty. \quad (B.2)$$

The right-hand side of (B.1) may be evaluated using the identity

$$\ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right) = \ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right) + \ln \left( \frac{E^\beta_\alpha}{E^\beta_\alpha - E^\beta_\alpha} \right)$$

$$\ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right) = \ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right) + \int_0^1 \mathrm{d} \alpha \left( \frac{D \beta}{E^\beta_\alpha - E^\beta_\alpha} \beta \right) \quad (B.3)$$

where the operator $D$ is defined such that

$$D \beta = E^\beta_\alpha \beta \quad \text{for bound states},$$

$$[D, \Lambda^B] = 0 = [D, \Lambda^C]. \quad (B.4)$$

Therefore, (B.1) may be rewritten as

$$\ln \left( \frac{h_\alpha^B}{\Delta^B_\alpha} \right) = \frac{1}{M^\alpha_B} \left\{ \langle \alpha| r^B_\alpha - r^\beta_\alpha | \beta \rangle \ln \left( \frac{h_\alpha^B}{E^B_\alpha - E^\beta_\alpha} \right) \right\}$$

$$+ \int_0^1 \mathrm{d} \alpha \left( \langle \alpha| r^B_\alpha - r^\beta_\alpha | \beta \rangle \right) \right\}, \quad (B.5)$$

where

$$\tilde{q}^B_\alpha = \left( \frac{1}{E^B_\alpha - E^D_\alpha} \right) B. \quad (B.6)$$

As in Sections II and III, we may now replace the $\Lambda^B_\alpha$ and $\tilde{q}^B_\alpha$ by their semiclassical approximations. That is,

$$\Lambda^B_\alpha \rightarrow \frac{1}{2 \beta^2} \sin^2 \left( \frac{\pi v}{2} \right) \quad (B.7)$$

and

$$\tilde{q}^B_\alpha \rightarrow \frac{1}{2 \beta^2} \int_0^p \frac{\beta^2 \sin^2 (\beta u)}{2 \beta^2 - 2 \beta^2 v} \, \mathrm{d} \beta \quad (B.8)$$

where $V(v)$ is the single-particle model potential defined in Sec. II. Similar expressions can be derived for $\Delta^C_\alpha$ by replacing in (B.5) the subspace label $B$ by $C$.

We do not consider (B.5) further in this paper, since $\Lambda^B_\alpha$ and $\Delta^C_\alpha$ appear in the cross sections only logarithmically so that their effect would not be expected to change the overall estimate of $\sigma$ in any serious way.
Research supported in part by the U. S. Atomic Energy Commission and by the Air Force Office of Scientific Research, Office of Aerospace Research, United States Air Force, under Contract #Fa4620-70-C-0028.

On sabbatical leave from the Physics Department, University of Connecticut, Storrs, Connecticut 06268. Participating guest, Lawrence Berkeley Laboratory.


5. For example, R. Latter, Phys. Rev. 99, 510 (1955); J. C. Stewart and M. Rotenberg, ibid A140, 1508 (1965).


9. Corrections for a relativistic impacting electron will be introduced later.

Table I. The parameter $d$ in the single-particle potential as given in Ref. 6. The same values are used for all $Z_I$ at each $Z_C$. (Atomic units.)

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Table II. The energy eigenvalues calculated with the single-particle model potential of Ref. 6, for the core charges $Z_C = 10, 20, 30, \text{ and } 40$. The values of $Z_I$ are chosen for all closed subshells. The energies $E_{n\ell}$ are given in Rydbergs.

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Table V. The transition probabilities and overlap integrals for \( Z_0 = 20 \), and in the dipole approximation. All values are given in atomic units. \( Z_1 \) denotes the degree of isolation.
Table VI. Comparison of the transition probabilities to the continuum as calculated here and those given in Ref. 8. $c_{nl}$ is defined by (2.13).

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Table VII. The ionization cross sections $\sigma^C$, $\sigma^A$, and $\sigma^I$ in units of $n^2 a_0^2$, where $a_0$ = Bohr radius. $\sigma^B$ corresponds to total excitation cross section to all the bound states, where the effect of the exclusion principle is neglected. The experimental values are summarized in Ref. 3.

\[ E_0 = 1 \text{ KeV}: \quad \sigma^B = 0.363 \]
\[ (n^2 a_0^2 \text{ unit}) \quad \sigma^C = 0.396 \]
\[ \sigma^A = 0.087 \]
\[ \sigma^I = 0.483 \quad \text{Exp.} \quad \sigma^I \approx 0.55 \sim 0.43 \]

\[ E_0 = 10 \text{ KeV}: \quad \sigma^B = 0.053 \]
\[ \sigma^C = 0.058 \]
\[ \sigma^A = 0.013 \quad \text{Exp.} \quad \sigma^I \approx 0.07 \]
\[ \sigma^I = 0.071 \]

\[ E = 20 \text{ MeV}: \quad \sigma^B = 0.0049 \]
\[ \sigma^C = 0.0083 \]
\[ \sigma^A = 0.0019 \]
\[ \sigma^I = 0.0102 \]
FIGURE CAPTIONS

Fig. 1. The transition probabilities \( M_D \) to all the allowed bound states and \( M_C \) to all the continuum, at \( Z_C = 30 \). The numbers next to each curve are \( (n\ell^+) \) or \( (n\ell^-) \). The solid lines are the \( M_D \) values, while the dotted lines are for \( M_C \).

Fig. 2. The relative Auger branching ratio as estimated from the fluorescence yield calculations.

Fig. 3. The estimated ionization cross sections \( \sigma^C \) and \( \sigma^A \) corresponding to the direct excitations to the continuum and the excitations to bound states followed by the Auger emissions, respectively. \( Z = Z_C - Z_I \), where \( Z_C \) is the core charge and \( Z_I \) is the degree of ionization of the target before the collision. All values are given in \( \pi a_0^2 \) units and the electron energy is 20 MeV. The solid lines are the values for \( \sigma^A \), while the dotted lines are for \( \sigma^C \).

Fig. 4. The total ionization cross sections for 20 Mev electron as functions of \( Z_C \) and \( Z = Z_C - Z_I \). All values are given in \( \pi a_0^2 \) units.
Fig. 1
Fig. 3

\( \sigma^C \) and \( \sigma^A \)

\( Z = Z_C - Z_I \)
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