

## Electron-impact excitation of electric octupole transitions in positive ions: Asymptotic behavior of the sum over partial-collision strengths

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An investigation has been made, for the case of octupole transitions, of the dependence of the partial-collision strength on the orbital angular momentum of the colliding electron. It is shown that, similar to the dipole and quadrupole transitions, the sum over partial-collision strengths is asymptotic to a geometric series of common ratio  $E_j/E_i$ , where  $E_i$  and  $E_j$  are the initial and final energies of the colliding electron, respectively. For large incident energies ( $E_j/E_i \sim 1$ ) the convergence of the sum to the geometric series is rather slow, since the geometric-series method only starts to become valid for large values of angular momentum. This difficulty is overcome by developing an alternative method in which the approximation is made that  $E_j/E_i = 1$ . An analytic formula is then obtained to estimate the contribution to the total-collision strength from large values of angular momentum. Results of partial- and total-collision strengths are presented for direct electric octupole transitions in  $\text{Ca}^+$  and  $\text{Sr}^+$ .

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### I. INTRODUCTION

Optically forbidden  $E3$ -type transitions in positive ions [1,2] may be excited by electron impact. It is already known that in the case of dipole [3,4] and quadrupole [5] transitions the sums of partial-collision strengths are asymptotic to a geometric series with common ratio  $E_j/E_i$ . The object of this paper is to show that octupole transitions follow the same pattern; and the sum of partial-collision strengths, for a colliding electron angular momentum  $l \gg E_j/(E_i - E_j)$ , is also asymptotic to a geometric series with the same common ratio  $E_j/E_i$ , where  $E_i$  and  $E_j$  are the initial and final energies of the colliding electron, respectively. As  $E_i$  increases, the ratio  $E_j/E_i \sim 1$  and the convergence of the sum to the geometric series is rather slow. In this case a different method is implemented to complete the sum. The approximation used in this procedure is  $E_j/E_i = 1$ , and consequently several expressions from the general theory of Coulomb excitation reduce appreciably. It is shown that for  $l$  large, terms in the infinite sum decrease as  $l^{-5}$ ,  $l^{-6}$ , and  $l^{-7}$ . The collision problem has been formulated in atomic units, except for energies where we have used Rydberg units.

### II. THEORY

The initial work closely follows that of a previous paper [5]. We give, without derivation, the expressions used in calculating the dimensionless quantity collision strength for electron-impact excitation of positive ions. The total-collision strength  $\Omega(nl_a \rightarrow n'l'_a)$  has the partial-wave expansion

$$\Omega(nl_a \rightarrow n'l'_a) = \sum_{l,l'} \Omega_{l'l} \quad (1)$$

where  $nl_a$  and  $n'l'_a$  are the initial and final target states, and  $l$  and  $l'$  are the initial and final quantum numbers for

the angular momentum of the colliding electron. The expression for  $\Omega_{l'l}$  in terms of the transmission matrix  $\underline{T}$  is given by

$$\Omega_{l'l} = \sum_{S=0,1} \sum_L \frac{1}{2} (2S+1) |T(n'l'_a k'l'LS, nl_a k l, LS)|^2 \quad (2)$$

where  $k$  and  $k'$  are the wave numbers of the incident and scattered electron, respectively, and  $L$  and  $S$  the conserved total angular momenta and total spin quantum number, respectively. The transmission matrix  $\underline{T}$  is of block-diagonal type with each block corresponding to a given  $LS$  symmetry for the total system (i.e., target ion plus colliding electron).

The infinite sum in Eq. (1) is split into two parts

$$\Omega(nl_a \rightarrow n'l'_a) = \Omega_{l_0} + \bar{\Omega}_{l_0+1} \quad (3)$$

where

$$\Omega_{l_0} = \sum_{l=0}^{l_0} \sum_{l'} \Omega_{l'l} \quad (4)$$

and

$$\bar{\Omega}_{l_0+1} = \sum_{l=l_0+1}^{\infty} \sum_{l'} \Omega_{l'l}^{\text{CBeI}} \quad (5)$$

The sum from  $l=0$  to  $l_0$  may be evaluated in any desired approximation, e.g.,  $R$ -matrix method, close coupling, Coulomb distorted wave, etc. The sum from  $l=l_0+1$  to  $\infty$  is estimated using the Coulomb Bethe weak-coupling approximation (CBeI) to the transmission matrix. In the limit of large  $l$  the ratio  $(\Omega_{l'l}/\Omega_{l'l}^{\text{CBeI}}) \sim 1$ , and then  $l_0$  is chosen so that this condition is fulfilled. Since relativistic effects have been neglected in the collision Hamiltonian and the effect of exchange between the colliding and bound electron is negligible when  $l_0$  is large, the transmission matrix  $\underline{T}$  does not depend on  $S$  and

$$\Omega_{l'l}^{\text{CBeI}} = 2 \sum_L (2L+1) |T^{\text{CBeI}}(n'l'_a k'l'L, nl_a k l, L)|^2 \quad (6)$$

Standard techniques of Racah algebra reduce the previous expression to

$$\begin{aligned} \Omega_{l'l'}^{\text{CBel}} &= 32(2l_a+1)(2l'_a+1)(2l+1)(2l'+1) \\ &\times \sum_{\lambda} \frac{(C_{000}^{l_a l'_a \lambda} C_{000}^{l l' \lambda})^2}{(2\lambda+1)^3} (z-1)^{2\lambda-2} \\ &\times B^2(nl_a, n'l'_a; \lambda) I^2(\kappa l, \kappa' l'; \lambda), \end{aligned} \quad (7)$$

where  $C_{000}^{l_a l'_a \lambda}$  and  $C_{000}^{l l' \lambda}$  are Clebsch-Gordan coefficients [6],  $\lambda$  satisfies the selection rules  $|l-l'| \leq \lambda \leq l+l'$  and  $|l_a-l'_a| \leq \lambda \leq l_a+l'_a$ , and  $(z-1)$  is the ion charge. The integral  $B(nl_a, n'l'_a; \lambda)$  is given by

$$B(nl_a, n'l'_a; \lambda) = \int_0^\infty P_{nl_a}(r) r^\lambda P_{n'l'_a}(r) dr, \quad (8)$$

where  $P_{nl_a}$  and  $P_{n'l'_a}$  are the radial wave functions of the initial and final states of the atomic system. Details regarding the numerical evaluation of these single orbital wave functions have been given elsewhere [5]. The Coulomb integrals  $I(\kappa l, \kappa' l'; \lambda)$  are defined as

$$I(\kappa l, \kappa' l'; \lambda) = \int_0^\infty \mathcal{F}(\kappa l | \rho) \mathcal{F}(\kappa' l' | \rho) \rho^{-\lambda-1} d\rho, \quad (9)$$

where

$$\mathcal{F}(\kappa l | \rho) = (z-1)^{1/2} F_{kl}(r) \quad (10)$$

and

$$\kappa = \frac{k}{(z-1)} \quad \text{and} \quad \rho = (z-1)r. \quad (11)$$

The Coulomb functions  $F_{kl}$  are subject to the boundary conditions

$$F_{kl}(0) = 0 \quad (12)$$

and

$$F_{kl}(r) \underset{r \rightarrow \infty}{\sim} k^{-1/2} \sin \left[ kr + \frac{(z-1)}{k} (2kr) - \frac{l\pi}{2} + \sigma_l \right], \quad (13)$$

with

$$\sigma_l = \arg \Gamma \left[ l + 1 - i \frac{(z-1)}{k} \right]. \quad (14)$$

### A. Electric-octupole- ( $E3$ -) type transitions

For transitions between target states involving  $\lambda \geq 3$  and considering only the lowest multiple order  $\lambda=3$ , Eq. (7) reduces to

$$\begin{aligned} \Omega_{l'l'}^{\text{CBel}} &= \frac{120}{7} (z-1)^4 B^2(nl_a, n'l'_a; 3) \\ &\times \frac{l_{a>}(l_{a>}-1)(l_{a>}-2)}{(2l_{a>}-1)(2l_{a>}-3)} \frac{(l_{>}+1)l_{>}(l_{>}-1)}{(2l_{>}-3)(2l_{>}+3)} \\ &\times I^2(\kappa l, \kappa' l'; 3), \quad l' = l \pm 1 \end{aligned} \quad (15)$$

and

$$\begin{aligned} \Omega_{l'l'}^{\text{CBel}} &= \frac{200}{7} (z-1)^4 B^2(nl_a, n'l'_a; 3) \\ &\times \frac{l_{a>}(l_{a>}-1)(l_{a>}-2)}{(2l_{a>}-1)(2l_{a>}-3)} \frac{l_{>}(l_{>}-1)(l_{>}-2)}{(2l_{>}-1)(2l_{>}+3)} \\ &\times I^2(\kappa l, \kappa' l'; 3), \quad l' = l \pm 3, \end{aligned} \quad (16)$$

where  $l_{a>}$  and  $l_{>}$  are the greater of  $l_a$  and  $l'_a$  and of  $l$  and  $l'$ , respectively.

Using Eqs. (15) and (16) in Eq. (5),  $\tilde{\Omega}_{l_0+1}$  reduces to

$$\begin{aligned} \tilde{\Omega}_{l_0+1} &= \frac{40}{7} (z-1)^4 B^2(nl_a, n'l'_a; 3) \\ &\times \frac{l_{a>}(l_{a>}-1)(l_{a>}-2)}{(2l_{a>}-1)(2l_{a>}+3)} S_{l_0+1}, \end{aligned} \quad (17)$$

where

$$\begin{aligned} S_{l_0+1} &= \sum_{l=l_0+1}^{\infty} \left[ 3 \frac{(l+1)l(l-1)}{(2l-3)(2l+3)} I^2(\kappa l, \kappa' l-1; 3) + 3 \frac{(l+2)(l+1)l}{(2l-1)(2l+5)} I^2(\kappa l, \kappa' l+1; 3) \right. \\ &\quad \left. + 5 \frac{l(l-1)(l-2)}{(2l-1)(2l-3)} I^2(\kappa l, \kappa' l-3; 3) + 5 \frac{(l+3)(l+2)(l+1)}{(2l+5)(2l+3)} I^2(\kappa l, \kappa' l+3; 3) \right]. \end{aligned} \quad (18)$$

### B. Limit of large orbital angular momentum

#### 1. Geometric-series method

In the limit of large angular momentum ( $l \gg 1$ ) the Coulomb integral becomes [7]

$$I(\kappa l, \kappa' l'; \lambda) \sim \exp \left[ \frac{\pi}{2} |\eta - \eta'| \right] I_0(\kappa l, \kappa' l'; \lambda), \quad (19)$$

where

$$\eta = \frac{1}{\kappa}, \quad \eta' = \frac{1}{\kappa'}, \quad (20)$$

and  $I_0(\kappa l, \kappa' l', \lambda)$  is the integral in Eq. (9) evaluated in the Born approximation. The radial wave functions  $\mathcal{F}(\kappa l | \rho)$  are in this case related to the spherical Bessel functions. The connection is given through the relation

$$\mathcal{F}(\kappa l | \rho) = \sqrt{\kappa} j_l(\kappa \rho) . \tag{21}$$

By employing the further relation

$$j_l(\kappa \rho) = \left[ \frac{\pi}{2\kappa \rho} \right]^{1/2} J_{l+1/2}(\kappa \rho) , \tag{22}$$

between the spherical Bessel functions and ordinary Bessel functions one obtains

$$I_0(\kappa l, \kappa' l'; \lambda) = \frac{\pi}{2} \int_0^\infty J_{l+1/2}(\kappa \rho) J_{l'+1/2}(\kappa' \rho) \rho^{-\lambda} d\rho . \tag{23}$$

The integral is of the Weber-Schafheitlin type and has a discontinuity in the expressions for  $I_0$  at  $\kappa = \kappa'$ . Using the analytic continuation of the  ${}_2F_1$  Gauss hypergeometric function given by

$${}_2F_1(a, b; c; w) = (1-w)^{-b} {}_2F_1\left(c-a, b; c; \frac{w}{w-1}\right) , \tag{24}$$

one readily finds from Watson [8] that for  $0 < \kappa' < \kappa$

$$I_0(\kappa l, \kappa' l'; \lambda) = \frac{\pi}{2^{\lambda+1}} \left[ \frac{\kappa'}{\kappa} \right]^{l'+1/2} \kappa^{\lambda-1} \left[ \frac{\kappa^2 - \kappa'^2}{\kappa^2} \right]^{-[(l'-l-\lambda+1)/2]} \frac{\Gamma((l+l'-\lambda+2)/2)}{\Gamma(l'+\frac{3}{2})\Gamma((l-l'+\lambda+1)/2)} \\ \times {}_2F_1\left[\frac{l'-l+\lambda+1}{2}, \frac{l'-l-\lambda+1}{2}; l'+\frac{3}{2}; \frac{\kappa'^2}{\kappa^2 - \kappa'^2}\right] , \tag{25}$$

and for  $0 < \kappa < \kappa'$

$$I_0(\kappa l, \kappa' l'; \lambda) = \frac{\pi}{2^{\lambda+1}} \left[ \frac{\kappa}{\kappa'} \right]^{l+1/2} \kappa'^{\lambda-1} \left[ \frac{\kappa'^2 - \kappa^2}{\kappa'^2} \right]^{-[(l-l'-\lambda+1)/2]} \frac{\Gamma((l+l'-\lambda+2)/2)}{\Gamma(l+\frac{3}{2})\Gamma((l'-l+\lambda+1)/2)} \\ \times {}_2F_1\left[\frac{l-l'+\lambda+1}{2}, \frac{l-l'-\lambda+1}{2}; l+\frac{3}{2}; \frac{\kappa^2}{\kappa'^2 - \kappa^2}\right] . \tag{26}$$

Substituting  $\lambda = 3$  into Eqs. (25) and (26) it is shown that

$$I_0(\kappa l, \kappa' l - 1; 3) = \frac{\pi}{16} \left[ \frac{\kappa <}{\kappa >} \right]^{l+1/2-p} \kappa^2 \left[ \frac{\kappa^2 - \kappa'^2}{\kappa^2} \right]^{1/2+p} \frac{\Gamma(l-1)}{\Gamma(l+\frac{3}{2}-p)\Gamma(\frac{3}{2}+p)} \\ \times {}_2F_1\left[\frac{5}{2}-p, -\frac{1}{2}-p; l+\frac{3}{2}-p; \frac{\kappa^2}{\kappa^2 - \kappa'^2}\right] , \tag{27}$$

$$I_0(\kappa l, \kappa' l + 1; 3) = \frac{\pi}{16} \left[ \frac{\kappa <}{\kappa >} \right]^{l+1/2+p} \kappa^2 \left[ \frac{\kappa^2 - \kappa'^2}{\kappa^2} \right]^{3/2-p} \frac{\Gamma(l)}{\Gamma(l+\frac{3}{2}+p)\Gamma(\frac{5}{2}-p)} \\ \times {}_2F_1\left[\frac{3}{2}+p, -\frac{3}{2}+p; l+\frac{3}{2}+p; \frac{\kappa^2}{\kappa^2 - \kappa'^2}\right] , \tag{28}$$

where

$$p = \begin{cases} 0 & \text{if } \kappa < \kappa' \\ 1 & \text{if } \kappa > \kappa' \end{cases} ,$$

and

$$I_0(\kappa l, \kappa' l - 3; 3) = \frac{\pi}{16} \left[ \frac{\kappa <}{\kappa >} \right]^{l+1/2-p} \kappa^2 \left[ \frac{\kappa^2 - \kappa'^2}{\kappa^2} \right]^{-1/2+p} \frac{\Gamma(l-2)}{\Gamma(l+\frac{3}{2}-p)\Gamma(\frac{1}{2}+p)} \\ \times {}_2F_1\left[\frac{7}{2}-p, \frac{1}{2}-p; l+\frac{3}{2}-p; \frac{\kappa^2}{\kappa^2 - \kappa'^2}\right] , \tag{29}$$

$$I_0(\kappa l, \kappa' l + 3; 3) = \frac{\pi}{16} \left[ \frac{\kappa_{<}}{\kappa_{>}} \right]^{l+1/2+p} \kappa_{>}^2 \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right]^{5/2-p} \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2}+p)\Gamma(\frac{7}{2}-p)} \\ \times {}_2F_1 \left[ \frac{1}{2} + p, -\frac{5}{2} + p; l + \frac{3}{2} + p; \frac{\kappa_{<}^2}{\kappa_{<}^2 - \kappa_{>}^2} \right] \quad (30)$$

where

$$p = \begin{cases} 0 & \text{if } \kappa < \kappa' \\ 3 & \text{if } \kappa > \kappa' \end{cases}.$$

$\kappa_{<}$  ( $\kappa_{>}$ ) is the smaller (greater) of  $\kappa$  and  $\kappa'$ . The behavior of  ${}_2F_1(a, b; c; w)$  for fixed  $a, b, w$ , and large  $|c|$  is described by

$${}_2F_1(a, b; c; w) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^m \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)n!} w^n + O(|c|^{-m-1}). \quad (31)$$

Using the previous asymptotic expansion and the limit property of the  $\Gamma$  function

$$\lim_{n \rightarrow \infty} n^{t-s} \frac{\Gamma(n+s)}{\Gamma(n+t)} = 1, \quad (32)$$

it is possible to show that, for excitation of octupole transitions ( $\kappa > \kappa'$ ) and  $l$  large ( $l \gg \kappa_{<}^2 / (\kappa_{>}^2 - \kappa_{<}^2) \equiv E_j / (E_i - E_j)$ ),  $l$ -dependent terms in Eq. (18) behave as

$$\frac{5l(l-1)(l-2)}{(2l-1)(2l-3)} I^2(\kappa_{>} l, \kappa_{<} l - 3; 3) \approx \frac{\pi}{720} \left[ \frac{\kappa_{<}}{\kappa_{>}} \right]^{2l-5} \kappa_{>}^4 \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right]^5 e^{\pi|\eta_{>} - \eta_{<}|}, \quad (33)$$

$$3 \frac{(l+1)l(l-1)}{(2l-3)(2l+3)} I^2(\kappa_{>} l, \kappa_{<} l - 1; 3) \approx \frac{\pi}{192} \left[ \frac{\kappa_{<}}{\kappa_{>}} \right]^{2l-1} \kappa_{>}^4 \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right]^3 l^{-2} e^{\pi|\eta_{>} - \eta_{<}|}, \quad (34)$$

$$3 \frac{(l+2)(l+1)l}{(2l-1)(2l+5)} I^2(\kappa_{>} l, \kappa_{<} l + 1; 3) \approx \frac{3\pi}{256} \left[ \frac{\kappa_{<}}{\kappa_{>}} \right]^{2l+3} \kappa_{>}^4 \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right] l^{-4} e^{\pi|\eta_{>} - \eta_{<}|}, \quad (35)$$

and

$$5 \frac{(l+3)(l+2)(l+1)}{(2l+5)(2l+3)} I^2(\kappa_{>} l, \kappa_{<} l + 3; 3) \approx \frac{5\pi}{1024} \left[ \frac{\kappa_{<}}{\kappa_{>}} \right]^{2l+7} \kappa_{>}^4 \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right]^{-1} l^{-6} e^{\pi|\eta_{>} - \eta_{<}|}. \quad (36)$$

Substituting Eqs. (33)–(36) into  $S_{l_0+1}$  [Eq. (18)] gives

$$S_{l_0+1} \sim \frac{\pi}{720} e^{\pi|\eta_{>} - \eta_{<}|} \frac{\kappa_{>}^9}{\kappa_{<}^5} \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{>}^2} \right]^5 \\ \times \sum_{l=l_0+1}^{\infty} \left[ \frac{\kappa_{<}^2}{\kappa_{>}^2} \right]^l \left[ 1 + \frac{15}{4} \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{<}^2} \right]^{-2} l^{-2} + \frac{135}{16} \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{<}^2} \right]^{-4} l^{-4} + \frac{225}{64} \left[ \frac{\kappa_{>}^2 - \kappa_{<}^2}{\kappa_{<}^2} \right]^{-6} l^{-6} \right] \quad (37)$$

and for  $l \gg \kappa_{<}^2 / (\kappa_{>}^2 - \kappa_{<}^2)^{-1}$  the infinite sum in  $S_{l_0+1}$  is asymptotic to a geometric series of ratio  $\kappa_{<}^2 / \kappa_{>}^2 \equiv E_j / E_i$ .

Therefore the main contribution to the sum over  $l$ , in Eq. (17), arises from the partial-collision strength  $\Omega_{l-3, l}^{\text{CBel}}(\kappa_{<}, \kappa_{>})$ . The completion of the summation over partial-collision strength is then straightforward and leads to the result

$$\tilde{\Omega}_{l_0+1} \sim \Omega_{l_0-2, l_0+1}^{\text{CBel}}(\kappa_{<}, \kappa_{>}) \frac{1}{(1-x)}, \quad l_0 \gg \frac{\kappa_{<}^2}{\kappa_{>}^2 - \kappa_{<}^2} \quad (38)$$

where

$$x = \frac{\kappa_{<}^2}{\kappa_{>}^2} = \frac{k_{<}^2}{k_{>}^2} = \frac{E_j}{E_i}, \quad (39)$$

and  $E_i$  and  $E_j$  are the energies of the free electron before and after the collision. For an  $s$ - $f$  transition the additional approximation is made that

$$\tilde{\Omega}_{l_0+1} \sim \Omega(nl_a \rightarrow n'l'_a; L = l_0 + 1) / (1-x). \quad (40)$$

## 2. The method of sum of reciprocal powers

For large incident energies, such as for, e.g.,  $E_j = 10.924\ 11$  Ry and a transition energy  $E_{ij} = E_i - E_j = 0.145\ 51$  Ry ( $5s-4f$  in  $\text{Ca}^+$ ),  $x = E_j/E_i = 0.987$  or  $E_j/(E_i - E_j) = 75$ , and the series method becomes impractical because this method is valid for partial waves  $l > l_0$ , where  $l_0 \gg E_j/(E_i - E_j) = 75$ . Numerical quantal calculations of partial waves [Eq. (4)] in the different approximations,  $R$ -matrix method, close coupling, Coulomb distorted wave, become prohibitive at such large values of  $l$ .

To obtain an estimate of  $S_{l_0+1}$ , at high incident electron energies, the approximation is made that  $\kappa = \kappa'$  and  $\bar{\kappa}^2 = (\kappa^2 + \kappa'^2)/2$ . In this case, the octupole integrals  $I(\kappa l, \kappa' l'; 3)$  in Eq. (18) simplify considerably [7] and reduce to

$$I(\bar{\kappa}l, \bar{\kappa}l + 1; 3) = \frac{\bar{\kappa}^3}{3l(l+1)(l+2)(2l+1)(2l+3)} [1 + \bar{\kappa}^2(l+1)^2]^{-1/2} \times \left[ \frac{6}{\bar{\kappa}^3} [1 + \bar{\kappa}^2(l+1)^2] \left[ \pi(1 - e^{-2\pi/\bar{\kappa}})^{-1} + \bar{\kappa}^3 \sum_{s=0}^l \frac{s^2}{1 + \bar{\kappa}^2 s^2} \right] - l(l+1)(2l+1) \right], \quad (41)$$

$$I(\bar{\kappa}l, \bar{\kappa}l - 1; 3) = \frac{\bar{\kappa}^3}{3(l-1)l(l+1)(2l-1)(2l+1)} [1 + \bar{\kappa}^2 l^2]^{-1/2} \times \left[ \frac{6}{\bar{\kappa}^3} (1 + \bar{\kappa}^2 l^2) \left[ \pi(1 - e^{-2\pi/\bar{\kappa}})^{-1} + \bar{\kappa}^3 \sum_{s=0}^l \frac{s^2}{1 + \bar{\kappa}^2 s^2} \right] - (l-1)l(2l-1) \right], \quad (42)$$

$$I(\bar{\kappa}l, \bar{\kappa}l + 3; 3) = \frac{\bar{\kappa}^5}{15[1 + \bar{\kappa}^2(l+1)^2]^{1/2}[1 + \bar{\kappa}^2(l+2)^2]^{1/2}[1 + \bar{\kappa}^2(l+3)^2]^{1/2}}, \quad (43)$$

$$I(\bar{\kappa}l, \bar{\kappa}l - 3; 3) = \frac{\bar{\kappa}^5}{15[1 + \bar{\kappa}^2(l-2)^2]^{1/2}[1 + \bar{\kappa}^2(l-1)^2]^{1/2}(1 + \bar{\kappa}^2 l^2)^{1/2}}. \quad (44)$$

These expressions may be further simplified if the assumption is made that  $l^2 \bar{\kappa}^2 \gg 1$  and

$$\sum_{s=0}^l \frac{s^2}{1 + \bar{\kappa}^2 s^2} \approx \frac{l}{\bar{\kappa}^2}.$$

The final expression obtained for  $S_{l_0+1}$  is

$$S_{l_0+1} \approx a_5(\bar{\kappa}) \sum_{l=l_0+1}^{\infty} \frac{1}{l^5} + a_6(\bar{\kappa}) \sum_{l=l_0+1}^{\infty} \frac{1}{l^6} + a_7(\bar{\kappa}) \sum_{l=l_0+1}^{\infty} \frac{1}{l^7}, \quad (45)$$

where

$$a_5(\bar{\kappa}) = \frac{8}{45} \bar{\kappa}^4, \quad (46)$$

$$a_6(\bar{\kappa}) = \frac{\bar{\kappa}^3 \pi}{2} (1 - e^{-2\pi/\bar{\kappa}})^{-1}, \quad (47)$$

$$a_7(\bar{\kappa}) = \frac{3}{8} \bar{\kappa}^2 \pi^2 (1 - e^{-2\pi/\bar{\kappa}})^{-2}. \quad (48)$$

The sums of reciprocal powers  $\sum_{l=l_0+1}^{\infty} l^{-p}$  with  $p = 5, 6, 7$  have been calculated using the relation

$$\sum_{l=l_0+1}^{\infty} l^{-p} = \zeta(p) - \sum_{l=1}^{l_0} l^{-p} \quad (49)$$

TABLE I. CDWII partial-collision strength  $\Omega_l$ , for the  $4s-4f$  and  $5s-4f$  transitions in  $\text{Ca}^+$ . Energy of the colliding electron after excitation  $E_j$  (Ry).

$E_j = 0.129\ 11$			$E_j = 1.226\ 31$			$E_j = 6.310\ 10$		
$l$	$4s-4f$	$5s-4f$	$l$	$4s-4f$	$5s-4f$	$l$	$4s-4f$	$5s-4f$
9	$1.514 \times 10^{-2}$	1.370	29	$5.984 \times 10^{-5}$	$4.012 \times 10^{-2}$	39	$2.644 \times 10^{-3}$	$1.037 \times 10^{-1}$
10	$3.406 \times 10^{-3}$	$9.000 \times 10^{-1}$	30	$3.912 \times 10^{-5}$	$3.380 \times 10^{-2}$	40	$2.318 \times 10^{-3}$	$9.246 \times 10^{-2}$
11	$6.986 \times 10^{-4}$	$5.182 \times 10^{-1}$	31	$2.560 \times 10^{-5}$	$2.860 \times 10^{-2}$	41	$2.036 \times 10^{-3}$	$8.258 \times 10^{-2}$
12	$1.344 \times 10^{-4}$	$2.746 \times 10^{-1}$	32	$1.676 \times 10^{-5}$	$2.428 \times 10^{-2}$	42	$1.791 \times 10^{-3}$	$7.386 \times 10^{-2}$
13	$2.484 \times 10^{-5}$	$1.383 \times 10^{-1}$	33	$1.098 \times 10^{-5}$	$2.066 \times 10^{-2}$	43	$1.578 \times 10^{-3}$	$6.618 \times 10^{-2}$
14	$4.466 \times 10^{-6}$	$6.752 \times 10^{-2}$	34	$7.198 \times 10^{-6}$	$1.765 \times 10^{-2}$	44	$1.392 \times 10^{-3}$	$5.938 \times 10^{-2}$
15	$7.908 \times 10^{-7}$	$3.234 \times 10^{-2}$	35	$4.720 \times 10^{-6}$	$1.511 \times 10^{-2}$	45	$1.230 \times 10^{-3}$	$5.338 \times 10^{-2}$
16	$1.390 \times 10^{-7}$	$1.531 \times 10^{-2}$	36	$3.098 \times 10^{-6}$	$1.297 \times 10^{-2}$	46	$1.088 \times 10^{-3}$	$4.808 \times 10^{-2}$
17	$2.420 \times 10^{-8}$	$7.196 \times 10^{-3}$	37	$2.036 \times 10^{-6}$	$1.116 \times 10^{-2}$	47	$9.642 \times 10^{-4}$	$4.338 \times 10^{-2}$
18	$4.192 \times 10^{-9}$	$3.368 \times 10^{-3}$	38	$1.337 \times 10^{-6}$	$9.618 \times 10^{-3}$	48	$8.554 \times 10^{-4}$	$3.922 \times 10^{-2}$
19	$7.252 \times 10^{-10}$	$1.572 \times 10^{-3}$	39	$8.788 \times 10^{-7}$	$8.306 \times 10^{-3}$	49	$7.596 \times 10^{-4}$	$3.552 \times 10^{-2}$
20	$1.262 \times 10^{-10}$	$7.320 \times 10^{-4}$	40	$5.780 \times 10^{-7}$	$7.186 \times 10^{-3}$	50	$6.752 \times 10^{-4}$	$3.224 \times 10^{-2}$
21	$2.178 \times 10^{-11}$	$3.408 \times 10^{-4}$	41	$3.802 \times 10^{-7}$	$6.228 \times 10^{-3}$	51	$6.008 \times 10^{-4}$	$2.930 \times 10^{-2}$

TABLE II. CDWII partial-collision strength  $\Omega_l$  for the  $5s-4f$  and  $6s-4f$  transitions in  $\text{Sr}^+$ . Energy of the colliding electron after excitation  $E_j$  (Ry).

$E_j=0.10513$			$E_j=1.20328$			$E_j=6.03514$		
$l$	$5s-4f$	$6s-4f$	$l$	$5s-4f$	$6s-4f$	$l$	$5s-4f$	$6s-4f$
9	$1.433 \times 10^{-2}$	1.424	29	$1.477 \times 10^{-4}$	$4.744 \times 10^{-2}$	39	$4.060 \times 10^{-3}$	$1.104 \times 10^{-1}$
10	$3.308 \times 10^{-3}$	$9.656 \times 10^{-1}$	30	$9.980 \times 10^{-5}$	$3.946 \times 10^{-2}$	40	$3.576 \times 10^{-3}$	$9.850 \times 10^{-1}$
11	$6.908 \times 10^{-4}$	$5.846 \times 10^{-1}$	31	$6.748 \times 10^{-5}$	$3.360 \times 10^{-2}$	41	$3.154 \times 10^{-3}$	$8.796 \times 10^{-2}$
12	$1.331 \times 10^{-4}$	$3.252 \times 10^{-1}$	32	$4.566 \times 10^{-5}$	$2.874 \times 10^{-2}$	42	$2.786 \times 10^{-3}$	$7.864 \times 10^{-2}$
13	$2.414 \times 10^{-5}$	$1.701 \times 10^{-1}$	33	$3.092 \times 10^{-5}$	$2.466 \times 10^{-2}$	43	$2.466 \times 10^{-3}$	$7.044 \times 10^{-2}$
14	$4.208 \times 10^{-6}$	$8.546 \times 10^{-2}$	34	$2.094 \times 10^{-5}$	$2.122 \times 10^{-2}$	44	$2.186 \times 10^{-3}$	$6.320 \times 10^{-2}$
15	$7.152 \times 10^{-7}$	$4.174 \times 10^{-2}$	35	$1.419 \times 10^{-5}$	$1.833 \times 10^{-2}$	45	$1.940 \times 10^{-3}$	$5.678 \times 10^{-2}$
16	$1.194 \times 10^{-7}$	$2.002 \times 10^{-2}$	36	$9.618 \times 10^{-5}$	$1.587 \times 10^{-2}$	46	$1.725 \times 10^{-3}$	$5.112 \times 10^{-2}$
17	$1.966 \times 10^{-8}$	$9.494 \times 10^{-3}$	37	$6.522 \times 10^{-6}$	$1.378 \times 10^{-2}$	47	$1.535 \times 10^{-3}$	$4.610 \times 10^{-2}$
18	$3.210 \times 10^{-9}$	$4.466 \times 10^{-3}$	38	$4.424 \times 10^{-6}$	$1.200 \times 10^{-2}$	48	$1.368 \times 10^{-3}$	$4.166 \times 10^{-2}$
19	$5.218 \times 10^{-10}$	$2.092 \times 10^{-3}$	39	$3.004 \times 10^{-6}$	$1.047 \times 10^{-2}$	49	$1.221 \times 10^{-3}$	$3.772 \times 10^{-2}$
20	$8.486 \times 10^{-11}$	$9.764 \times 10^{-4}$	40	$2.040 \times 10^{-6}$	$9.156 \times 10^{-3}$	50	$1.090 \times 10^{-3}$	$3.420 \times 10^{-2}$
21	$1.355 \times 10^{-11}$	$4.548 \times 10^{-4}$	41	$1.385 \times 10^{-6}$	$8.024 \times 10^{-3}$	51	$9.750 \times 10^{-4}$	$3.106 \times 10^{-2}$

where  $\zeta(p)$  is the Riemann zeta function. The calculations were carried out using the symbolic computation program MAPLE [9], to a high degree of accuracy. Hereafter  $S_{l_0+1}$  [Eq. (45)] is inserted into Eq. (17) to yield  $\tilde{\Omega}_{l_0+1}$ .

### III. RESULTS

Results are presented for two optically forbidden  $E3$ -type transitions in  $\text{Ca}^+$  and  $\text{Sr}^+$ . Collision strengths were obtained using a unitarized nonexchange Coulomb-distorted-wave (CDWII) seven-state approximation,  $4s-3d-4p-5s-4d-5p-4f$  in  $\text{Ca}^+$  and  $5s-4d-5p-6s-5d-6p-4f$  in  $\text{Sr}^+$ . The target valence orbitals  $P_{n_l a}(r)$  are solutions of a one-electron Schrödinger equation with observed binding energies [10]. The collision approximation assumes  $LS$  coupling and takes into account all open channels based on the lowest seven states of  $\text{Ca}^+$  and  $\text{Sr}^+$ , respectively. Tables I and II contain partial-collision strengths for the excitation of the  $4s-4f$ ,  $5s-4f$  transitions in  $\text{Ca}^+$  and  $5s-$

$4f$ ,  $6s-4f$  transitions in  $\text{Sr}^+$ , respectively. The asymptotic behavior of the collision strengths for large angular momenta was checked using the data in Tables I and II. In Tables III and IV the ratio  $\Omega_l/\Omega_{l-1}$  has been tabulated as a function of the colliding electron angular momentum  $l$ , where  $\Omega_l = \sum_{l'} \Omega_{l'}$  for different energies of the colliding electron after excitation. For large  $l$ ,  $\Omega_l^{\text{CDWII}} \sim \Omega_{l'}^{\text{CPeI}}$  and the ratio  $\Omega_l/\Omega_{l-1}$  tends to a constant  $x = E_j/E_i$ , where  $E_i$  and  $E_j$  are the energies of the free electron before and after excitation. Tables III and IV show results for the excitation of the  $4s-4f$  and  $5s-4f$  transitions in  $\text{Ca}^+$  and excitation of the  $5s-4f$  and  $6s-4f$  transitions in  $\text{Sr}^+$ , respectively. Also shown are the quantities  $x = E_j/E_i$  and  $a = E_j/(E_i - E_j)$ . These tables illustrate the fact that for large values of the electron-impact energy, and/or for transitions in which the atomic states are energetically close, e.g., the transition  $5s-4f$  in  $\text{Ca}^+$  and the transition  $6s-4f$  in  $\text{Sr}^+$ , the sum over partial-collision strengths  $\tilde{\Omega}_{l_0+1}$  [Eq. (5)] is slowly convergent, to a geometric series of common ratio  $E_j/E_i$ . The

TABLE III.  $\Omega_l/\Omega_{l-1}$  for the  $4s-4f$  and  $5s-4f$  transitions in  $\text{Ca}^+$ .  $x = E_j/E_i$ ,  $a = E_j/E_{ij}$ . Energy of the colliding electron before excitation  $E_i$  (Ry), energy of the colliding electron after excitation  $E_j$  (Ry). Excitation energy  $E_{ij}(\text{Ry}) = E_i - E_j$ .

$E_j=0.12911$			$E_j=1.22631$			$E_j=631010$		
$l$	$x=0.172$ $a \sim 0.2$ $4s-4f$	$x=0.470$ $a \sim 0.9$ $5s-4f$	$l$	$x=0.664$ $a \sim 2$ $4s-4f$	$x=0.894$ $a \sim 8$ $5s-4f$	$l$	$x=0.910$ $a \sim 10$ $4s-4f$	$x=0.978$ $a \sim 43$ $5s-4f$
10	0.225	0.657	30	0.654	0.842	40	0.877	0.892
11	0.205	0.576	31	0.654	0.846	41	0.878	0.893
12	0.192	0.530	32	0.655	0.849	42	0.879	0.894
13	0.185	0.504	33	0.655	0.851	43	0.881	0.896
14	0.180	0.488	34	0.656	0.854	44	0.882	0.897
15	0.177	0.479	35	0.656	0.856	45	0.883	0.899
16	0.176	0.474	36	0.656	0.858	46	0.885	0.901
17	0.174	0.470	37	0.657	0.860	47	0.886	0.902
18	0.173	0.468	38	0.657	0.862	48	0.887	0.904
19	0.173	0.467	39	0.657	0.864	49	0.888	0.906
20	0.174	0.466	40	0.658	0.865	50	0.889	0.908
21	0.173	0.466	41	0.658	0.867	51	0.890	0.909

TABLE IV.  $\Omega_l/\Omega_{l-1}$  for the  $5s-4f$  and  $6s-4f$  transitions in  $Sr^+$ .  $x = E_j/E_i$ ,  $a = E_j/E_{ij}$ . Energy of the colliding electron before excitation  $E_i$  (Ry), energy of the colliding electron after excitation  $E_j$  (Ry). Excitation energy  $E_{ij}(\text{Ry}) = E_i - E_j$ .

$l$	$E_j = 0.105\ 13$		$l$	$E_j = 1.203\ 28$		$l$	$E_j = 6.035\ 14$	
	$x = 0.160$	$x = 0.470$		$x = 0.685$	$x = 0.910$		$x = 0.916$	$x = 0.981$
	$a \sim 0.2$	$a \sim 0.9$		$a \sim 2$	$a \sim 10$		$a \sim 11$	$a \sim 51$
	$5s-4f$	$6s-4f$		$5s-4f$	$6s-4f$		$5s-4f$	$6s-4f$
10	0.231	0.678	30	0.676	0.832	40	0.881	0.892
11	0.209	0.605	31	0.676	0.851	41	0.882	0.893
12	0.193	0.556	32	0.677	0.855	42	0.883	0.894
13	0.181	0.523	33	0.677	0.858	43	0.885	0.896
14	0.174	0.502	34	0.677	0.861	44	0.886	0.897
15	0.170	0.488	35	0.678	0.864	45	0.888	0.898
16	0.167	0.480	36	0.678	0.866	46	0.889	0.900
17	0.165	0.474	37	0.678	0.868	47	0.890	0.902
18	0.163	0.470	38	0.678	0.870	48	0.891	0.904
19	0.163	0.468	39	0.679	0.873	49	0.892	0.905
20	0.163	0.467	40	0.679	0.874	50	0.893	0.907
21	0.160	0.466	41	0.679	0.876	51	0.894	0.908

TABLE V. CDWII total-collision strength  $\Omega$  for the  $5s-4f$  transition in  $Sr^+$ . The contributions  $\Omega_{l_0}$  and  $\tilde{\Omega}_{l_0+1}$  to  $\Omega$  are shown separately.  $\tilde{\Omega}_{l_0+1}$  has been calculated using the geometric-series method.

$E_j$ (Ry)	$l_0$	$\Omega_{l_0}$	$\tilde{\Omega}_{l_0+1}$	$\Omega$	$\tilde{\Omega}_{l_0+1}$ as percentage of $\Omega$
0.105 13	20	1.278	$\sim 0$	1.278	$\sim 0$
0.214 94	20	1.328	$\sim 0$	1.328	$\sim 0$
0.462 83	20	1.362	$\sim 0$	1.362	$\sim 0$
1.203 28	40	1.346	$2.223 \times 10^{-6}$	1.346	$\sim 0$
1.642 54	40	1.293	$3.831 \times 10^{-5}$	1.293	$\sim 0$

TABLE VI. CDWII total-collision strength  $\Omega$  for the  $5s-4f$  transition in  $Ca^+$ . The contributions  $\Omega_{l_0}$  and  $\tilde{\Omega}_{l_0+1}$  to  $\Omega$  are shown separately, together with error estimates.  $\tilde{\Omega}_{l_0+1}$  has been calculated using the reciprocal power method.

$E_j$ (Ry)	$E_j/E_i$	$l_0$	$\Omega_{l_0}^{CDWII}/\Omega_{l_0}^{CBeI}$	$\Omega_{l_0}$	$\tilde{\Omega}_{l_0+1}$	$\Omega$	$\tilde{\Omega}_{l_0+1}$ as percentage of $\Omega$	Percentage absolute error in $\Omega$
6.310 10	0.977	51	0.94	14.704	$3.160 \times 10^{-1}$	15.020	2	1
10.924 11	0.987	59	1.08	14.406	$5.180 \times 10^{-1}$	14.924	3	1

TABLE VIII. Electric octupole integral  $B(ns, nf; 3)$ .

	Transition	$B(a_0^4)$
Ca <sup>+</sup>	4s-4f	-86.56
	5s-4f	712.2
Sr <sup>+</sup>	5s-4f	115.0
	6s-4f	-770.0

geometric-series method only starts to become useful for  $l > l_0$ , where  $l_0 \gg a = E_j / (E_i - E_j)$  and  $\Omega_{l_0}$  [Eq. (4)] then requires contributions from a large number of partial waves  $\Omega_{l'}$  which are calculated in any desired quantal approximation. For colliding energies near threshold, i.e.,  $0.10513 \leq E_j \leq 1.64254$  Ry,  $l_0$  has been chosen as the value at which  $\Omega_{l_0}^{\text{CDWII}} / \Omega_{l_0-1}^{\text{CDWII}} \sim x = E_j / E_i$  within at most a 4% error. In Table V, it is shown, for the transition 5s-4f in Sr<sup>+</sup>, for each incident electron energy and angular momentum  $l_0$ , the two contributions  $\Omega_{l_0}$  (CDWII approximation) and  $\tilde{\Omega}_{l_0+1}$  to the total-collision strength  $\Omega$ , as well as the percentage contribution to  $\tilde{\Omega}_{l_0+1}$ . The quantal calculations become increasingly difficult, from the computational point of view, as the electron-impact energy and  $l$  increase. Therefore, to avoid these difficulties, the alternative method of sums of reciprocal powers [Eq. (45)] is used to estimate  $S_{l_0+1}$ .

A sample calculation, on the 5s-4f transition in Ca<sup>+</sup>, of the contributions  $\Omega_{l_0}$  and  $\tilde{\Omega}_{l_0+1}$  to the total collision strength  $\Omega$  is presented in Table VI. The percentage contribution of  $\tilde{\Omega}_{l_0+1}$  to  $\Omega$  is also shown, as well as an estimate of the percentage error in  $\Omega$  due to the use of the analytic formulas (17) and (45), found by the method described below. The error estimate is only for this effect, not for the CDWII approximation which is of the order of 1%. An upper bound on the average error made by using  $\tilde{\Omega}_{l_0+1}$  to complete the infinite sum may be estimated in the following way. The contribution to  $\Omega$  from angular momentum  $l_1 + 1$  to  $l_2$  is denoted by  $\Delta\Omega$  and is calculated by two methods. The first estimate is

$$\Delta\Omega^{\text{num}} = \sum_{l=l_1+1}^{l_2} \sum_{l'} \Omega_{l'l}^{\text{CDWII}},$$

which has been compared with the second estimate

$$\Delta\Omega = \tilde{\Omega}_{l_1+1} - \tilde{\Omega}_{l_2+1},$$

which uses the approximate formulas (17) and (45). It has been then assumed that the error thus found in  $\Delta\Omega$  is constant for all  $\tilde{\Omega}_l$  when  $l > l_2$ . This is clearly an overestimate of the total error, because Eqs. (17) and (45) represent better the contribution to the total-collision strength  $\Omega$  from large angular momentum, as  $l$  increases. The percentage error in  $\Omega$  is obtained by dividing the percentage error in  $\tilde{\Omega}_{l_0}$  by  $\Omega$ . The procedure to estimate this error is similar to the one developed for quadrupole transitions [11]. At the largest impact energy  $E_j = 22.46911$  Ry, and for the transitions 5s-4f in Ca<sup>+</sup> and 6s-4f in Sr<sup>+</sup>, an estimate of the error is more difficult since the convergence of the CDWII to the CBeI approximation has not been attained at an angular momentum as large as  $l = 58$ . These data points were not included in Table IX. In order to show that the geometric-series method does not give accurate results for the energies listed in Table VI, the contribution  $\tilde{\Omega}_{l_0+1}$  that the method would give is presented in Table VII, together with the contribution  $\Omega_{l_0}$ . The percentage contribution of  $\tilde{\Omega}_{l_0+1}$  to  $\Omega$  is also shown, as well as an estimate of the percentage error in  $\Omega$  due to the use of formula (40). Because the contribution of  $\tilde{\Omega}_{l_0+1}$  to  $\Omega$  is so large for  $E_j = 22.46911$  Ry, the scheme used to calculate the percentage error in  $\Omega$  no longer applies and the error shown is undoubtedly too low. Values of the electric octupole integral  $B(ns; nf; 3)$  [Eq. (8)] are shown in Table VIII for both ions.

Total-collision strengths, for excitation of octupole transitions in Ca<sup>+</sup> and Sr<sup>+</sup>, obtained using a unitarized seven-state CDWII approximation are given in Table IX, including values at  $E_j = \infty$  obtained by the Born approximation.

In the limit of infinite electron-impact energy, the Born approximation for the collision strength of an electric oc-

TABLE IX. CDWII total-collision strengths  $\Omega(ns, n'f)$  for Ca<sup>+</sup> and Sr<sup>+</sup>. Energy of the colliding electron after excitation  $E_j$  (Ry). Transition energy  $E_{ij}$  (Ry) =  $E_i - E_j$ .

$E_j$	Ca <sup>+</sup>		Sr <sup>+</sup>		
	4s-4f $E_{ij} = 0.62089$	5s-4f $E_{ij} = 0.14551$	$E_j$	5s-4f $E_{ij} = 0.55376$	6s-4f $E_{ij} = 0.11850$
0.12911	2.184	15.596	0.10513	2.556	16.132
0.38510	2.144	17.052	0.21494	2.656	17.646
0.76451	2.026	16.908	0.46283	2.724	18.196
1.22631	1.918	16.358	1.20328	2.692	17.046
1.69343	1.828	15.900	1.64254	2.586	16.746
6.31010	1.411	15.020	6.03514	2.126	15.638
10.92411	1.298	14.924	10.42774	2.020	15.530
22.46911	1.218		21.40924	1.947	
$\infty$	1.193	14.872	$\infty$	1.936	15.477



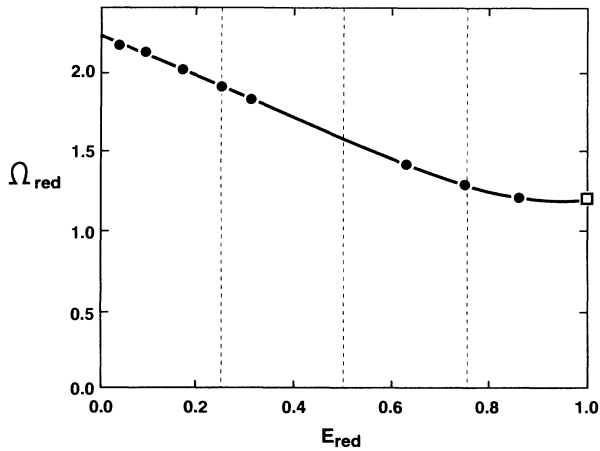


FIG. 1. Scaled total-collision strength  $\Omega_{\text{red}}$  for the  $4s-4f$  transition in  $\text{Ca}^+$ , plotted against scaled energy  $E_{\text{red}}$ .  $\bullet$ , reduced data; —, spline fit to the reduced data;  $\square$ , Born limit. Adjustable parameter  $C=4$  with knot values 2.238, 1.919, 1.572, 1.290, 1.193.

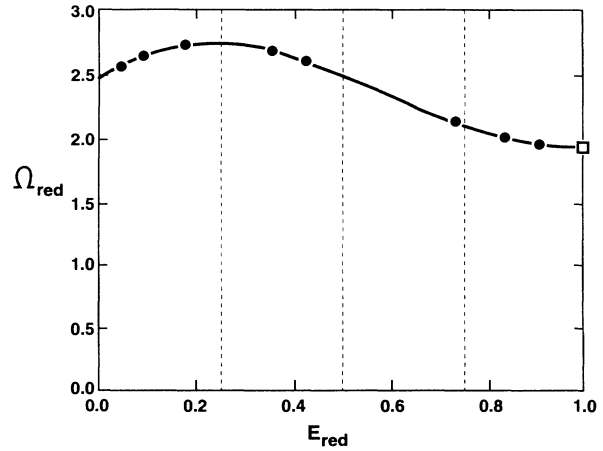


FIG. 3. Scaled total-collision strength  $\Omega_{\text{red}}$  for the  $5s-4f$  transition in  $\text{Sr}^+$ , plotted against scaled energy  $E_{\text{red}}$ .  $\bullet$ , reduced data; —, spline fit to the reduced data;  $\square$ , Born limit. Adjustable parameter  $C=6$  with knot values 2.465, 2.75, 2.481, 2.095, 1.934.

tupole transition between  $nl_a - n'l'_a$  levels can be written as

$$\Omega = C_3 I_3^{(-3)}, \quad (50)$$

where the factor  $C_3 = 112$  depends only on the quantum numbers of the transition in question and  $I_3^{(-3)}$  is an integral over momentum transfer given by

$$I_3^{(-3)} = \int_0^\infty \left[ \int_0^\infty P_{nl_a} P_{n'l'_a} j_3(Kr) dr \right]^2 K^{-3} dK, \quad (51)$$

and where  $j_3(Kr)$  is a spherical Bessel function of the first kind.

In order to interpolate the data in Table IX, use has been made of the interactive graphics program OMEUPS

which is based on the method by Burgess and Tully [12] for interpolating and compacting collision strengths. Summaries of the method and the program are given elsewhere [13–15]. The originality of the method hinges on the use of scaling techniques which remove the main energy dependence from the data and map the entire range of  $E$  onto the interval  $[0,1]$ . The scaled or reduced variables are denoted by  $E_{\text{red}}$ ,  $\Omega_{\text{red}}$ . For an optically forbidden transition the data are reduced as

$$E_{\text{red}} = (E_i/E_{ij}) / (E_j/E_{ij} + C), \quad (52)$$

$$\Omega_{\text{red}} = \Omega, \quad (53)$$

where  $C > 0$  and  $E_j = E_i - E_{ij}$  is the free-electron energy

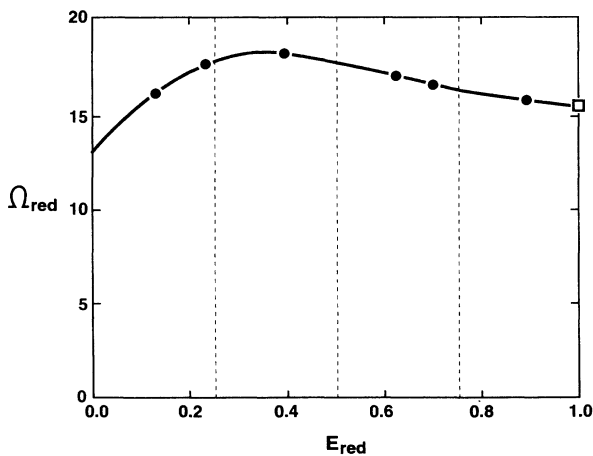


FIG. 2. Scaled total-collision strength  $\Omega_{\text{red}}$  for the  $5s-4f$  transition in  $\text{Ca}^+$ , plotted against scaled energy  $E_{\text{red}}$ .  $\bullet$ , reduced data; —, spline fit to the reduced data;  $\square$ , Born limit. Adjustable parameter  $C=4$  with knot values 13.04, 17.78, 17.88, 16.32, 15.46.

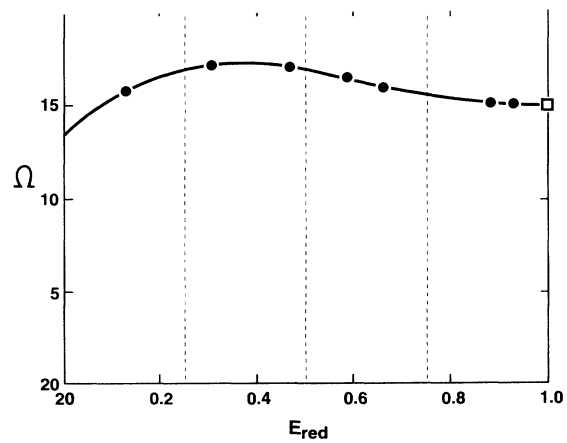


FIG. 4. Scaled total-collision strength  $\Omega_{\text{red}}$  for the  $6s-4f$  transition in  $\text{Sr}^+$ , plotted against scaled energy  $E_{\text{red}}$ .  $\bullet$ , reduced data; —, spline fit to the reduced data;  $\square$ , Born limit. Adjustable parameter  $C=6$  with knot values 13.26, 16.81, 16.77, 15.45, 14.87.

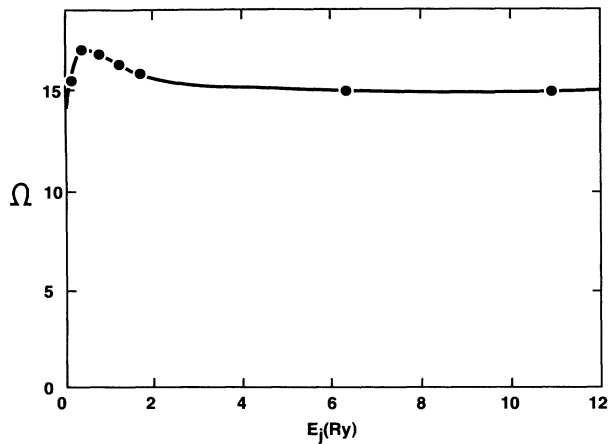


FIG. 5. Total-collision strength  $\Omega$  for the  $5s-4f$  transition in  $\text{Ca}^+$ , plotted against electron energy after excitation  $E_j$ . ●, original data; —, spline fit to the data.

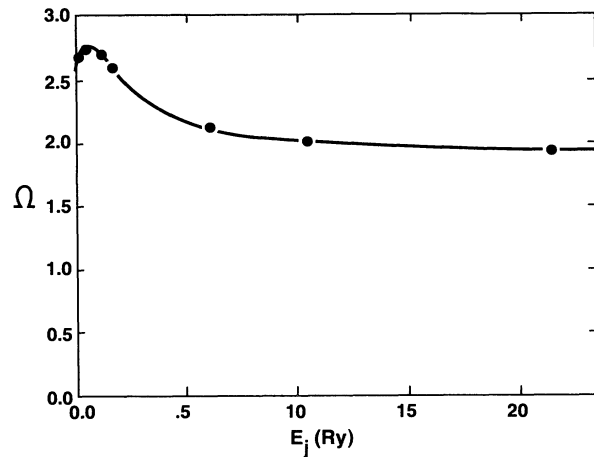


FIG. 6. Total-collision strength  $\Omega$  for the  $5s-4f$  transition in  $\text{Sr}^+$ , plotted against electron energy after excitation  $E_j$ . ●, original data; —, spline fit to the data.

after excitation. The parameter  $C$  depends on the transition; its value can be adjusted in order to optimize the plot of  $\Omega_{\text{red}}$  prior to making a spline fit. The spline curve is defined by its values at the five equally spaced knots. A short program for the spline interpolation and extrapolation is given in Appendix C of a previous publication [13]. Figures 1–4 are examples, produced by an IBM PS/2 of the reduced data and spline fit to the reduced data for the  $s-f$  transitions in  $\text{Ca}^+$  and  $\text{Sr}^+$ . A graphical comparison of the original data ( $\Omega$ ) and the spline fit, which represents the data typically to an accuracy of a fraction of a percent, is shown in Figs. 5 and 6. It is worth mentioning that, for the transition  $5s-4f$  in  $\text{Ca}^+$ , the interpolation procedure of OMEUPS gives a collision strength of  $\Omega = 14.88$  for the energy point  $E_j = 22.46911$  Ry as compared to  $\Omega = 15.06$  shown in Table VI.

#### IV. CONCLUSIONS

The convergence of the sum over partial-collision strengths, for excitation of octupole transitions in positive ions, has been examined formally and by sample calculations on  $\text{Sr}^+$  and  $\text{Ca}^+$ . Two different methods, based on the Coulomb-Bethe approximation, were obtained to complete the summation over the infinite partial-wave contributions. The first method, referred to as the geometric-series method, makes use of the findings in this

paper, shared by dipole and quadrupole transitions, that the sum over partial-collision strengths is asymptotic to a geometric series of ratio  $E_j/E_i$ , where  $E_i$  and  $E_j$  are the initial and final energies of the colliding electron, respectively. The second method or method of sums of reciprocal powers, avoids the numerical difficulties encountered at large colliding electron energies ( $E_j/E_i \sim 1$ ) when the convergence of the sum to the geometric series is rather slow.

These methods have been incorporated into the calculation of total-collision strengths for electron-impact excitation of  $s-f$  transitions in  $\text{Sr}^+$  and  $\text{Ca}^+$  ions. These total-collision strengths, calculated in the nonexchange Coulomb-distorted-wave approximation CDWII, have been analyzed using the OMEUPS method which removes the main energy dependence from the data and maps the entire range onto the interval  $[0,1]$ . The OMEUPS method also verifies that the analytic formulas derived to estimate the contribution to the total-collision strength from large values of angular momentum give data with the correct high-energy behavior.

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