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Excitation of positive ions in Coulomb-Born approximation

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We have presented a method for the evaluation of the Coulomb-Born matrix element between arbitrary initial and final Slater orbitals. Since for the two- or more-electron ionic target the wave functions may be constructed by the combination of the Slater orbitals of various angular momenta, one can easily apply this method to calculate the cross sections for the electron-impact excitation of a complex ion from an arbitrary initial state to an arbitrary final state. As an example we have calculated the excitation cross sections of the He^+ ion from the ground state to the $4f$ state at several energies.

INTRODUCTION

In recent years much attention has been focused on intensive studies of the excitation of positive ions under electron impact. Tully[1] has calculated the excitation cross sections of a number of one-electron ions in the Coulomb-Born (CB) approximation up to the d state and it is worthwhile to extend the investigation to higher—angular momentum states. Moreover, in a complex ionic system with two or more electrons, one may construct the target wave functions both for the initial and the final channels by combining the Slater orbitals of various angular momenta. These are the facts that motivated us to study the excitation of positive ions from an arbitrary initial Slater orbital to an arbitrary final Slater orbital in the CB approximation. This investigation is thus equally applicable in simple as well as complex ionic systems.

THEORY

To calculate the matrix element between arbitrary initial and final Slater orbitals in the CB approximation, we need to evaluate integrals of the type

$$I=\int\int e^{-\lambda r_1} r_1^{n+l_1+l_2} Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_1)\frac{1}{r_{12}} \times \chi_i(\vec{r}_2)\chi_f^*(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 , \quad (1)$$

where χ_i and χ_f are the Coulomb wave functions for the initial and final states.

Using the expression[2] for the product of two spherical harmonics appearing in Eq. (1), I can be obtained in terms of the integrals of the type

$$J=\int J_1(\vec{r}_2)\chi_i(\vec{r}_2)\chi_f^*(\vec{r}_2)d\vec{r}_2 , \quad (2)$$

where

$$J_1(\vec{r}_2)=\int \frac{e^{-\lambda r_1}}{r_{12}} r_1^{N+L} Y_{LM}(\hat{r}_1)d\vec{r}_1 . \quad (3)$$

Since

$$\int e^{-\lambda r_1} r_1^{L-1} Y_{LM}(\hat{r}_1) e^{i\vec{K}\cdot\vec{r}_1} d\vec{r}_1 = 4\pi(2i)^L L! \frac{K^L Y_{LM}(\hat{K})}{(\lambda^2+K^2)^{L+1}} , \quad (4)$$

then using the back Fourier-transform formula, we can write

$$e^{-\lambda r_1} r_1^{L-1} Y_{LM}(\hat{r}_1) = \frac{4\pi(2i)^L L!}{(2\pi)^3}\int \frac{K^L Y_{LM}(\hat{K})}{(\lambda^2+K^2)^{L+1}} e^{-i\vec{K}\cdot\vec{r}_1} d\vec{K} . \quad (5)$$

Substituting Eq. (5) in Eq. (3) we obtain

$$J_1(\vec{r}_2)=4\pi\left[-\frac{\partial}{\partial\lambda}\right]^{N+1}\frac{4\pi(2i)^L L!}{(2\pi)^3} \times \int \frac{K^L Y_{LM}(\hat{K})}{K^2(\lambda^2+K^2)^{L+1}} e^{-i\vec{K}\cdot\vec{r}_2} d\vec{K} . \quad (6)$$

Using the Feynman identity

$$\frac{1}{a^m b^n}=\frac{(m+n-1)!}{(m-1)!(n-1)!}\int_0^1 \frac{x^{m-1}(1-x)^{n-1}}{[ax+b(1-x)]^{m+n}}dx$$

with $a=\lambda^2+K^2$, $b=K^2$, $m=L+1$, and $n=1$ we get, writing $\mu_1=\lambda\sqrt{x}$,

$$J_1(\vec{r}_2)=2\pi\left[-\frac{\partial}{\partial\lambda}\right]^{N+1}\int_0^1\left[-\frac{\partial}{\mu_1\partial\mu_1}\right]\left[\frac{4\pi(2i)^L L!}{(2\pi)^3}\int\frac{K^L Y_{LM}(\hat{K})}{(\mu_1^2+K^2)^{L+1}}e^{-i\vec{K}\cdot\vec{r}_2}d\vec{K}\right]x^L dx . \quad (7)$$

Making use of Eq. (5) and performing the differentiation with respect to μ_1 we obtain

$$J_1(\vec{r}_2)=2\pi\left[-\frac{\partial}{\partial\lambda}\right]^{N+1}\int_0^1 \frac{e^{-\lambda\sqrt{x}r_2}}{\lambda} r_2^L Y_{LM}(\hat{r}_2)x^{L-1/2}dx \;.$$

Applying the Leibniz theorem for the differentiation of a product we have

$$J_1(\vec{r}_2)=2\pi\int_0^1\left[\sum_{s=0}^{N+1}\frac{(N+1)!}{s!\lambda^{N+2-s}}e^{-\mu_1 r_2}r_2^{L+s}Y_{LM}(\hat{r}_2)\right]x^{L+s/2-1/2}dx \;. \tag{8}$$

We now substitute Eq. (8) in Eq. (2) and obtain

$$J=2\pi\int_0^1\sum_{s=0}^{N+1}\frac{(N+1)!}{s!\lambda^{N+2-s}}\left[-\frac{1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}\left[\int e^{-\mu r_2}r_2^{L+s}Y_{LM}(\hat{r}_2)e^{i\vec{q}\cdot\vec{r}_2}d\vec{r}_2\right]p(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2\right]$$
$$\times x^{L+s/2-1/2}dx \;, \tag{9}$$

where $\mu=\mu_1-iK_it_1-iK_ft_2$ and $\vec{q}=\vec{K}_i(1-t_1)-\vec{K}_f(1-t_2)$.

In deriving Eq. (9) we have used the following integral representation[3] for the confluent hypergeometric function appearing in χ_i and χ_f:

$${}_1F_1(i\alpha_j,1;z)=\frac{1}{2\pi i}\oint_{\Gamma_j}dt_j p(\alpha_j,t_j)e^{zt_j}$$

with

$$p(\alpha_j,t_j)=t_j^{i\alpha_j-1}(t_j-1)^{-i\alpha_j},\;\; j=1,2 \;.$$

The integration over r_2 in Eq. (9) can now be performed with the help of Eq. (4):

$$J=2\pi\int_0^1\sum_{s=0}^{N+1}\frac{(N+1)!}{s!\lambda^{N+2-s}}\left[-\frac{\partial}{\partial\mu}\right]^{s+1}\left[-\frac{4\pi(2i)^L L!}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}\frac{q^L Y_{LM}(\hat{q})}{(\mu^2+q^2)^{L+1}}p(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2\right]x^{L+s/2-1/2}dx \;. \tag{10}$$

The $(s+1)$th-order differentiation with respect to μ in Eq. (10) is then converted into a series of differentiations with respect to μ^2 by using the formula of Todd *et al.*[4] The differentiation with respect to μ^2 can be carried out easily and we arrive at

$$J=8\pi^2 i^L\int_0^1\sum_{s=0}^{N+1}\frac{(N+1)!}{s!\lambda^{N+2-s}}\sum_{r'=0}^{[(s+1)/2]}\frac{(-1)^{r'}2^{s+L+1-2r'}(s+1)!(s+L+1-r')!}{(s+1-2r')!r'!}$$
$$\times\left[-\frac{1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}\frac{q^L Y_{LM}(\hat{q})\mu^{s+1-2r'}}{(\mu^2+q^2)^{s+L+2-r'}}p(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2\right]x^{L+2/s-1/2}dx \;, \tag{11}$$

where $[(s+1)/2]$ represents the largest integer $\leq(s+1)/2$.

We now consider an integral of the type

$$H=\frac{-1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}\frac{\mu^A q^L Y_{LM}(\hat{q})}{(\mu^2+q^2)^B}p(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2 \tag{12}$$

with $B\geq A+L$. Here μ, q, and (μ^2+q^2) are linear functions of t_1 and t_2. Using the addition theorem of regular solid harmonics (see Ref. 5) we get, after choosing our axis of quantization along the direction of $\vec{K}_i$,

$$q^L Y_{LM}(\hat{q})=\sum_{l'=0}^{L}N_{l'l''}(t_1-l)^{l'}(t_2-1)^{l''} \;, \tag{13}$$

where

$$N_{l'l''}=\left[\frac{4\pi(2L+1)(L+M)!(L-M)!}{(2l'+1)(2l''+1)(l'!)^2(l''+M)!(l''-M)!}\right]^{1/2}(-1)^{l'}K_i^{l'}K_f^{l''}Y_{l'0}(\hat{K}_i)Y_{l''M}(\hat{K}_f) \;,$$

where $l''=L-l'$.

Also, we can write

$$\mu^A=\sum_{r=0}^{A}\sum_{s_1=0}^{A-r}\frac{(-i)^{r+s_1}A!\mu_1^{A-r-s_1}(K_it_1)^r(K_ft_2)^{s_1}}{r!s_1!(A-r-s_1)!} \tag{14}$$

and

$$(\mu^2+q^2)^{-B}=E^{-B}\sum_{u=0}^{\infty}\frac{(B)_u}{u!}\left[\frac{Ft_1}{E}\right]^u , \tag{15}$$

where $E=X-Yt_2$, $F=U-Vt_2$ with

$$\begin{aligned} &X=\mu_1^2+K_i^2+K_f^2-2\vec{K}_i\cdot\vec{K}_f,\quad Y=2(i\mu_1K_f+K_f^2-\vec{K}_i\cdot\vec{K}_f) ,\\ &U=2(i\mu_1K_i+K_i^2-\vec{K}_i\cdot\vec{K}_f),\quad V=-2(K_iK_f+\vec{K}_i\cdot\vec{K}_f) , \end{aligned} \tag{16}$$

and $(B)_u$ is the Pochhammer symbol

$$(B)_u=B(B+1)(B+2)\cdots(B+u-1),\quad (B)_0=1\ (u=0,1,2,\dots) .$$

Making use of Eqs. (13)—(15) we arrive at

$$H=\sum_{l'=0}^{L}N_{l'l''}\sum_{r=0}^{A}\sum_{s_1}^{A-r}\frac{(-i)^{r+s_1}A!\mu_1^{A-r-s_1}K_i^rK_f^{s_1}}{r!s_1!(A-r-s_1)!} \times\left[\frac{1}{2\pi i}\oint_{\Gamma_2}t_2^{s_1-1+i\alpha_2}(t_2-1)^{l''-i\alpha_2}E^{-B}\sum_{u=0}^{\infty}\frac{(B)_u}{u!}\left[\frac{F}{E}\right]^u\left[\frac{1}{2\pi i}\oint_{\Gamma_1}t_1^{r+u-1+i\alpha_1}(t_1-1)^{l'-i\alpha_1}dt_1\right]dt_2\right] . \tag{17}$$

Now using the results

$$\begin{aligned} &\frac{1}{2\pi i}\oint_{\Gamma}t^{P-1+i\alpha}(t-1)^{W-i\alpha}dt=\frac{(-1)^W(i\alpha)_P(1-i\alpha)_W}{(P+W)!} ,\\ &(C+D)!=C!(C+1)_D,\ \text{and}\ (T)_{C+D}=(T)_C(T+C)_D , \end{aligned} \tag{18}$$

we get from Eq. (17)

$$H=\sum_{l'=0}^{L}N_{l'l''}\sum_{r=0}^{A}\sum_{s_1=0}^{A-r}\frac{(-1)^{l'}(-i)^{r+s_1}A!\mu_1^{A-r-s_1}K_i^rK_f^{s_1}(1-i\alpha_1)_{l'}(i\alpha_1)_r}{r!s_1!(A-r-s_1)!(r+l')!} \times\left[\frac{1}{2\pi i}\oint_{\Gamma_2}t_2^{s_1-1+i\alpha_2}(t_2-1)^{l''-i\alpha_2}E^{-B}\sum_{u=0}^{\infty}\frac{(B)_u(i\alpha_1+r)_u}{u!(r+l'+1)_u}\left[\frac{F}{E}\right]^u dt_2\right] . \tag{19}$$

The infinite summation within the t_2 integral represents a Gaussian hypergeometric function ${}_2F_1(a,b,c;z)$ with $a=B$, $b=i\alpha_1+r$, $c=r+l'+1$, and $z=F/E$. Since $c-a$ in our case is a negative integer we can write (see Ref. 6)

$${}_2F_1\left[B,i\alpha_1+r,r+l'+1;\frac{F}{E}\right]=\frac{\Gamma(r+l'+1)\Gamma(B-r-i\alpha_1)}{\Gamma(B)\Gamma(l'+1-i\alpha_1)}\left[\frac{E-F}{E}\right]^{-r-i\alpha_1} \times\sum_{v=0}^{m'}\frac{(i\alpha_1+r)_v(-m')_v}{v!(i\alpha_1+r+1-B)_v}\left[\frac{E}{E-F}\right]^v , \tag{20}$$

where $-m'=r+l'+1-B$, m' being a positive integer.

Substitution of Eq. (20) into Eq. (19) gives us

$$H=\sum_{l'=0}^{L}N_{l'l''}\sum_{r=0}^{A}\sum_{s_1=0}^{A-r}\frac{(-1)^{l'}(-i)^{r+s_1}A!\mu_1^{A-r-s_1}K_i^rK_f^{s_1}(1-i\alpha_1)_{l'}(i\alpha_1)_r\Gamma(B-r-i\alpha_1)}{r!s_r!(A-r-s_1)!\Gamma(B)\Gamma(l'+1-i\alpha_1)} \times\sum_{v=0}^{m'}\frac{(i\alpha_1+r)_v(-m')_v}{v!(i\alpha_1+r+1-B)_v}\left[\frac{1}{2\pi i}\oint_{\Gamma_2}t_2^{s_1-1+i\alpha_2}(t_2-1)^{l''-i\alpha_2} \times E^{-(B-r-v-i\alpha_1)}(E-F)^{-(r+v+i\alpha_1)}dt_2\right] . \tag{21}$$

We now consider the evaluation of the contour integral

$$G=\frac{1}{2\pi i}\oint_{\Gamma_2}t_2^{s_1-1+i\alpha_2}(t_2-1)^{l''-i\alpha_2}E^{-Q}(E-F)^{-R}dt_2 , \tag{22}$$

where $Q=B-r-v-i\alpha_1$ and $R=r+v+i\alpha_1$. Expanding E^{-Q} and $(E-F)^{-R}$ in an infinite power series of t_2 we obtain

$$G=X^{-Q}X_1^{-R}\sum_{s_2=0}^{\infty}\sum_{s_3=0}^{\infty}\frac{(Q)_{s_2}(R)_{s_3}(Y/X)^{s_2}(Y_1/X_1)^{s_3}}{s_2!s_3!}\left[\frac{1}{2\pi i}\oint_{\Gamma_2}t_2^{s_1+s_2+s_3-1+i\alpha_2}(t_2-1)^{l''-i\alpha_2}dt_2\right] \quad (23)$$

with $X_1=X-U$ and $Y_1=Y-V$, where X, Y, U, and V are given in Eq. (16).

With the help of the results in Eq. (18) we can write

$$G=\frac{(-1)^{l''}X^{-Q}X_1^{-R}(i\alpha_2)_{s_1}(1-i\alpha_2)_{l''}}{(s_1+l'')!}\sum_{s_2=0}^{\infty}\sum_{s_3=0}^{\infty}\frac{(Q)_{s_2}(R)_{s_3}(i\alpha_2+s_1)_{s_2+s_3}}{s_2!s_3!(s_1+l''+1)_{s_2+s_3}}\left[\frac{Y}{X}\right]^{s_2}\left[\frac{Y_1}{X_1}\right]^{s_3}. \quad (24)$$

The double infinite summation in Eq. (24) represents an Appell hypergeometric function of two variables, $F_1(a,b_1,b_2,c;z_1,z_2)$ with $a=i\alpha_2+s_1$, $b_1=Q$, $b_2=R$, $c=s_1+l''+1$, $z_1=Y/X$, and $z_2=Y_1/X_1$. Here we see that

$$c-(b_1+b_2)=-m'' ,$$

m'' being a positive integer. Thus we may write (see Ref. 7)

$$F_1(i\alpha_2+s_1,Q,R,s_1+l''+1;Y/X,Y_1/X_1)=(1-Y_1/X_1)^{-\alpha}F_1(\alpha,\beta,-m'',\gamma;\epsilon_1,\epsilon_2) , \quad (25)$$

where $\alpha=i\alpha_2+s_1$, $\beta=Q$, $\gamma=s_1+l''+1$,

$$\epsilon_1=\frac{Y_1/X_1-Y/X}{Y_1/X_1-1}, \text{ and } \epsilon_2=\frac{Y_1/X_1}{Y_1/X_1-1} .$$

Now if we take the expansion of the F_1 function on the right-hand side of Eq. (25) in powers of ϵ_2 we see that the series will terminate and each term will be a ${}_2F_1$ function. Thus we finally obtain

$$G=\frac{(-1)^{l''}X^{-Q}X_1^{-R}(i\alpha_2)_{s_1}(1-i\alpha_2)_{l''}(1-Y_1/X_1)^{-\alpha}}{(s_1+l'')!}\sum_{h=0}^{m''}\frac{(\alpha)_h(-m'')_h(\epsilon_2)^h}{h!(\gamma)_h}\,{}_2F_1(\alpha+h,\beta,\gamma+h;\epsilon_1) . \quad (26)$$

Equations (26), (21), and (11) give us the matrix element I in Eq. (1) as a one-dimensional integral over x ranging from 0 to 1 which is to be evaluated numerically.

It is to be noted that the first and third parameters of the ${}_2F_1$ functions appearing in Eq. (26) increase gradually by unity up to a certain limit. This fact can be exploited with advantage for the evaluation of the series. We need not calculate all the ${}_2F_1$ functions. If we calculate only two such successive functions, the others can be obtained from these two by repeated use of contiguous relations for the ${}_2F_1$ functions.

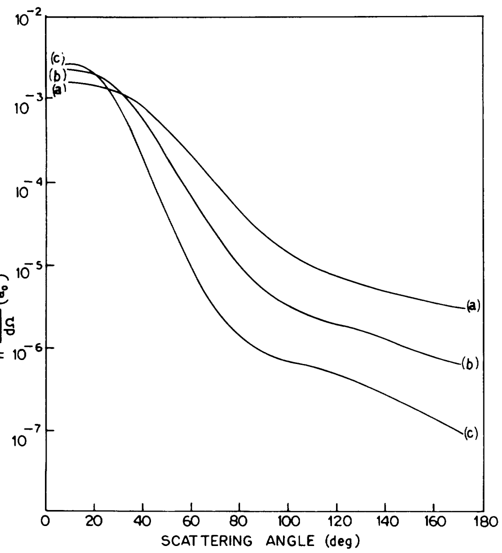

FIG. 1. Scaled differential cross sections $n^3d\sigma/d\Omega$, for $1s$-$4f$ excitation of the He^+ ion by electron impact in Coulomb-Born approximation at energies (a) 1.5, (b) 2, and (c) 3 times the threshold.

RESULTS AND DISCUSSIONS

For a consistency check we have reproduced by this method, our earlier results[8] for $1s$-$3p$ and $1s$-$4p$ excitation cross sections of the He^+ ion in the Coulomb-Born approximation. Next we applied this method to calculate the excitation cross section of the He^+ ion from the ground state to the $4f$ state. The one-dimensional integrals, with respect to the Feynman parameter have been evaluated by using the Gaussian quadrature formula, and suitable contiguous relations for the ${}_2F_1$ functions have been used for considerable reduction of computation time without affecting the accuracy of the results.

In Fig. 1 we have plotted the n^3 differential cross section (DCS) for the excitation of the He^+ ion from ground

TABLE I. Scaled total cross section (σn^3Z^4 in units of πa_0^2) for $1s$-$4f$ excitation of the He^+ ion by electron impact in Coulomb-Born approximation. Figures in brackets indicate the power of 10 by which the corresponding value is to be multiplied.

Energy in unit of threshold energy	Total scaled cross section in units of πa_0^2
1.5	1.5504(−2)
2	1.3907(−2)
3	1.0413(−2)
4	8.0754(−3)
6	5.5129(−3)

state to the $4f$ state against the scattering angle at incident energies 1.5, 2, and 3 times the threshold (n being the principle quantum number for the final state). It should be noted that with the increase of energy the DCS increases at small angles but decreases at large angles. Also, the DCS falls off as the scattering angle increases, at all energies. However, the rate of fall for a lower-energy curve is smaller than that for a higher-energy one.

In Table I we have tabulated the scaled total cross section $\sigma_{sc}=n^3Z^4\sigma$, at 1.5, 2, 3, 4, and 6 times the threshold energy (Z being the nuclear charge for the target ion).

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