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# Analytic expressions of radial integral on multiple transitions for Coulomb–Born approximation

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**Abstract**

The analytic expression for the two-electron integral of electron–ion scattering is re-examined carefully in terms of Appell's functions and Horn's functions. We study several analytic formulae in order to find actual programming code for the multipole transitions on electron–ion collisions.

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## 1. Introduction

A cross section accuracy of better than 20% for electron impact excitation of ions is desired for various applications in fusion research, astrophysics and atmospheric physics. So far, many elaborate calculations have been carried out for ionic stages by using methods such as the close-coupling calculation or the $R$-matrix method. However, the Coulomb–Born and Coulomb–Born–Oppenheimer approximations [1] are still useful methods for estimating the cross sections for high incident energies. Nakazaki [2] and Takagishi *et al* [3] presented radial integrals, which were expressed in terms of hypergeometric functions in the Coulomb–Born calculations of the excitation of positive ions by electron impact. They obtain expressions for the monopole and dipole terms only. Other multipole integrals are necessary to obtain various excitation cross sections, such as quadrapole transitions. Alder *et al* [4] have studied nuclear structures by an electromagnetic excitation with accelerated ions. For excitations of higher multipole orders, they showed the matrix elements involving the scattering states of the projectile can be expressed in terms of generalized hypergeometric functions of two variables, the so-called Appell function $F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y)$. Unfortunately, the analytic expression of the radial integral cannot be applied directly for Coulomb scattering because the convergence condition $|x| + |y| < 1$ of the Appell function does not hold. Swamy *et al* [5] studied the symmetry properties of the nonrelativistic Coulomb field problem and derived some relationship between radial integrals with respect to the multipole operator $r^{-q}$. Ramaker [6] described how to evaluate the seven basic one-centre two-electron integrals

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without the reduction of the matrix elements. He pointed out the seven different integrals could be evaluated by a single method in terms of a somewhat similar triple series:

$$S(\alpha, \alpha', \beta, \beta', \gamma, \gamma'; x, y, z) = \sum_{\lambda,\nu,\upsilon} \frac{\alpha'_\lambda \alpha_{\nu+\upsilon} \beta_\upsilon \beta'_{\lambda+\upsilon}}{\gamma_\upsilon \gamma'_{\lambda+\upsilon} \lambda! \nu! \upsilon!} x^\nu y^\upsilon z^\lambda.$$

He then presented a general expansion for $F_2(\alpha, \beta, \beta', \gamma, \gamma', x, y)$ in terms of the Appell function $F_1(a, b, b', c, y, y/(1-x))$. However, his method cannot be applied directly when $|y| > 1$ or $|y/(1-x)| > 1$ because the arguments $a$, $b$ and $b'$ become complex numbers in the present case, and the convergence condition for each $F_1$ function does not hold. Ancarani and Hervieux [7] studied the recurrence formulae and the WKB approximations for the Coulomb integrals.

The purpose of the present paper is to express the radial integrals in the Coulomb–Born approximation in terms of analytic expressions, which are valid for various incident energies and any partial wave, for the multipole transitions where the atomic radial functions are represented analytically as a linear combination of Slater type orbitals. The present method is applied to obtain the radial integrals, which are necessary to obtain the cross sections for the 2s → 3p, 2s → 3d and 2p → 3d transitions with $O^{7+}$. The present results are compared with others which are evaluated numerically.

## 2. The radial matrix elements for Coulomb scattering

In electron–ion scattering theory, one must evaluate the radial Coulomb integral, such as

$$M_{l_f l_i}^{-\lambda-1,q} = \frac{1}{k_f k_i} \int_0^\infty F_{l_f}(k_f r) r^{-\lambda-1} \exp(-qr) F_{l_i}(k_i r)\, dr \tag{1}$$

where the function $F_l(kr)$ is the regular Coulomb wave function for angular momentum $l$, wave number $k$ and $q \geqslant 0$:

$$F_l(kr) = \frac{|\Gamma(l+1+i\eta)|}{2\Gamma(2l+2)} e^{-\eta\pi/2} (2kr)^{l+1} e^{-ikr} {}_1F_1(l+1-i\eta, 2l+2, 2ikr). \tag{2}$$

Alder *et al* [4] obtained the analytic expression for the radial Coulomb integral as follows:

$$\begin{aligned} M_{l_i l_f}^{-\lambda-1,q} = & \frac{|\Gamma(l_i+1+i\eta_i)||\Gamma(l_f+1+i\eta_f)|}{(2l_i+1)!(2l_f+1)!} (l_i+l_f-\lambda+1)! \\ & \times i^{l_i+l_f-\lambda+2} x^{l_i} (-y)^{l_f} e^{-(\eta_i+\eta_f)\pi/2} (k_i - k_f + iq)^{\lambda-2} \\ & \times F_2(l_i+l_f-\lambda+2, l_i+1+i\eta_i, l_f+1-i\eta_f, 2l_i+2, 2l_f+2; x, y) \end{aligned} \tag{3}$$

where $\eta_\nu$ is the Sommerfeld parameter $(Z-1)/k_\nu$ ($\nu = $ i or f) for the nuclear charge $Z$ of the target ion and

$$\xi = \eta_f - \eta_i \qquad \eta_\nu = \frac{Z-1}{k_\nu} \qquad x = \frac{2\eta_f}{\xi + iq\eta_i/k_f} \qquad y = \frac{-2\eta_i}{\xi + iq\eta_i/k_f}. \tag{4}$$

Then they obtained several useful analytic expressions as a finite sum of terms each involving Appell's functions $F_2$ and $F_3$ for $q = 0$. Unfortunately, their most general expression in equation (IIB.62) of [4] has some errors. Therefore we re-examine the radial integral and derive the more general expression ($q \geqslant 0$), which leads to the correct limit at $q = 0$. The variables $x$ and $y$ are dependent on the incident energy, the Coulomb phase and $q$. For $q > 0$, some cases, such as $|x| > 1 > |y|$, arise for particular $q$ if the collision energy is fixed; the expressions in terms of the Appell functions $F_2$ and $F_3$ cannot be evaluated directly. Ramaker [6] pointed out that Appell's function $F_3(\alpha, \alpha', \beta, \beta', \gamma; x, y)$ should be expressed by a sum of two Horn functions $H_2(\alpha, \beta, \gamma, \delta, \epsilon; x, y)$ if either one of the arguments $x$ and $y$

was large and the remaining argument was small. Then he stated the transformation between $F_3$ and $H_2$. However, his transformation is not applicable, since one of the pre-factors of the Horn function $H_2$ becomes proportional to $\Gamma(-2l_\mathrm{f} - 1)$. Further deduction must be required. Therefore we present new analytic formulae for the equation (1) in terms of $F_2$ and $H_2$.

### *2.1. General expression for* $|x|, |y| > 1$

Equation (3) cannot be reduced to a single Appell function $F_1$ if $|l_\mathrm{i} - l_\mathrm{f}| \neq \lambda$. Thus Alder *et al* used the analytic continuation formula of $F_2$ as follows:

$$\begin{aligned}
&F_2(l_\mathrm{i}+l_\mathrm{f}-\lambda+2, l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, 2l_\mathrm{f}+2; x, y)\\
&\quad= \frac{\Gamma(-l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i})\Gamma(-l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f})\Gamma(\lambda-l_\mathrm{i}-l_\mathrm{f}-1)}{\Gamma(\lambda+1+\mathrm{i}\xi)\Gamma(-2l_\mathrm{i}-1)\Gamma(-2l_\mathrm{f}-1)}(-x)^{-l_\mathrm{i}-1+\mathrm{i}\eta_\mathrm{i}}(-y)^{-l_\mathrm{f}-1-\mathrm{i}\eta_\mathrm{f}}\\
&\qquad\times F_3(l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f}, -l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f}, \lambda+1+\mathrm{i}\xi; 1/x, 1/y)\\
&\qquad-\frac{\Gamma(2l_\mathrm{f}+1)\Gamma(-l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f})\Gamma(\lambda-l_\mathrm{i}-l_\mathrm{f}-1)}{\Gamma(-2l_\mathrm{f}-1)\Gamma(l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f})\Gamma(\lambda-l_\mathrm{i}+l_\mathrm{f})}(-y)^{-2l_\mathrm{f}-1}\\
&\qquad\times F_2(l_\mathrm{i}-l_\mathrm{f}+1-\lambda, l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, -2l_\mathrm{f}; x, y)\\
&\qquad-\frac{\Gamma(2l_\mathrm{i}+1)\Gamma(-l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i})\Gamma(\lambda-l_\mathrm{i}-l_\mathrm{f}-1)}{\Gamma(-2l_\mathrm{i}-1)\Gamma(l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i})\Gamma(\lambda-l_\mathrm{f}+l_\mathrm{i})}(-x)^{-2l_\mathrm{i}-1}\\
&\qquad\times F_2(l_\mathrm{f}-l_\mathrm{i}+1-\lambda, -l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f}, -2l_\mathrm{i}, 2l_\mathrm{f}+2; x, y)\\
&\qquad-\frac{\Gamma(2l_\mathrm{i}+1)\Gamma(2l_\mathrm{f}+1)\Gamma(\lambda-l_\mathrm{i}-l_\mathrm{f}-1)\Gamma(-l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i})\Gamma(-l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f})}{\Gamma(-2l_\mathrm{i}-1)\Gamma(-2l_\mathrm{f}-1)\Gamma(l_\mathrm{i}+l_\mathrm{f}+\lambda+1)\Gamma(l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i})\Gamma(l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f})}\\
&\qquad\times(-x)^{-2l_\mathrm{i}-1}(-y)^{-2l_\mathrm{f}-1}F_2(-l_\mathrm{i}-l_\mathrm{f}-\lambda, -l_\mathrm{i}-\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}+\mathrm{i}\eta_\mathrm{f}, -2l_\mathrm{i}, -2l_\mathrm{f}; x, y).
\end{aligned} \tag{5}$$

The signs of the coefficients with the $F_2$ functions on the right-hand side are different from equation (IIB.61) of [4] because Alder's original equation has the wrong signs; equation (5) can be derived from Alder's original formula (IIE.99) of [4].

This equation is singular for integer values of $l_\mathrm{i}$ and $l_\mathrm{f}$. Therefore Alder *et al* assumed $l_\mathrm{i}$ and $l_\mathrm{f}$ to have noninteger values while preserving $l_\mathrm{i} - l_\mathrm{f}$ as an integer. The third $F_2$ function can be eliminated by considering the complex conjugate equation to (5), which contains the same $F_2$ functions, according to the following Kummer type transformation [4, 8]:

$$\begin{aligned}
F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y) &= (1-x-y)^{-\alpha}\\
&\quad\times F_2(\alpha, \gamma-\beta, \gamma'-\beta', \gamma, \gamma'; x/(x+y-1), y/(x+y-1)).
\end{aligned} \tag{6}$$

After this elimination, one must take the limit of $l_\mathrm{i}, l_\mathrm{f}$ approaching integer values. Then we obtain the following expression for the radial matrix element:

$$\begin{aligned}
M_{l_\mathrm{i}l_\mathrm{f}}^{-\lambda-1,q} &= x^{-l_\mathrm{i}-1}(-y)^{l_\mathrm{f}}\frac{|\Gamma(l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f})|(2l_\mathrm{i})!}{|\Gamma(l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i})|(2l_\mathrm{f}+1)!(\lambda+l_\mathrm{i}-l_\mathrm{f}-1)!}\mathrm{i}^{l_\mathrm{i}-l_\mathrm{f}+\lambda-1}\\
&\quad\times(k_\mathrm{i}-k_\mathrm{f}+\mathrm{i}q)^{\lambda-2}\frac{\pi\mathrm{e}^{\xi\pi/2}}{\sinh\pi\xi}\\
&\quad\times F_2(l_\mathrm{f}-l_\mathrm{i}+1-\lambda, -l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}, -2l_\mathrm{i}, 2l_\mathrm{f}+2; x, y) + x^{l_\mathrm{i}}(-y)^{-l_\mathrm{f}-1}\\
&\quad\times\frac{|\Gamma(l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i})|(2l_\mathrm{f})!}{|\Gamma(l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f})|(2l_\mathrm{i}+1)!(\lambda-l_\mathrm{i}+l_\mathrm{f}-1)!}\mathrm{i}^{-l_\mathrm{i}+l_\mathrm{f}+\lambda+1}\\
&\quad\times(k_\mathrm{i}-k_\mathrm{f}+\mathrm{i}q)^{\lambda-2}\frac{\pi\mathrm{e}^{-\xi\pi/2}}{\sinh\pi\xi}\\
&\quad\times F_2(l_\mathrm{i}-l_\mathrm{f}+1-\lambda, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, -2l_\mathrm{f}; x, y)
\end{aligned}$$

$$+\mathrm{i}^{l_\mathrm{i}+l_\mathrm{f}+\lambda}x_\mathrm{i}^{l}(-y)^{l_\mathrm{f}}\frac{|\Gamma(l_\mathrm{f}+1+\mathrm{i}\eta_\mathrm{f})|}{|\Gamma(l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i})|}\frac{2\pi\,\mathrm{e}^{-(\eta_\mathrm{i}+\eta_\mathrm{f})\pi/2}}{\sinh\pi\xi}$$
$$\times(k_\mathrm{i}-k_\mathrm{f}+\mathrm{i}q)^{\lambda-2}(1-x-y)^{-(l_\mathrm{i}+l_\mathrm{f}-\lambda+2)/2}\mathbb{R}\Bigg\{\mathrm{i}(1-x-y)^{(l_\mathrm{i}+l_\mathrm{f}-\lambda+2)/2}$$
$$\times\frac{\Gamma(l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f})}{\Gamma(l_\mathrm{i}+1-\mathrm{i}\eta_\mathrm{i})\Gamma(\lambda+1-\mathrm{i}\xi)}(-x)^{-l_\mathrm{i}-1-\mathrm{i}\eta_\mathrm{i}}(-y)^{-l_\mathrm{f}-1+\mathrm{i}\eta_\mathrm{f}}$$
$$\times F_3(l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i},l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f},-l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i},-l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f},\lambda+1-\mathrm{i}\xi;1/x,1/y)\Bigg\}$$
$$|l_\mathrm{i}-l_\mathrm{f}|\neq\lambda. \tag{7}$$

In order to obtain good convergence in the series expansion of the functions $F_2$ and $F_3$, we use the Kummer type transformation [4, 8]:

$$F_2(\alpha,\beta,\beta',\alpha,\alpha;x,y)=(1-x)^{-\beta}(1-y)^{-\beta'}{}_2F_1(\beta,\beta',\alpha;xy/(1-x)(1-y)) \tag{8}$$
$$F_2(\alpha,\beta,\beta',\gamma,\alpha;x,y)=(1-y)^{-\beta'}F_1(\beta,\alpha-\beta',\gamma;x,x/(1-y)) \tag{9}$$
$$F_1(\alpha,\beta,\beta',\gamma;x,y)=(1-y)^{-\beta'}F_3(\alpha,\gamma-\alpha,\beta,\beta',\gamma;x,-y/(1-y)). \tag{10}$$

For the case $l_\mathrm{i}=l_\mathrm{f}\pm\lambda$, and $l_\mathrm{f}=l$, the Appell function $F_2$ in equation (3) can be written as follows:

$$F_2(2l+2,l\pm\lambda+1+\mathrm{i}\eta_\mathrm{i},l+1-\mathrm{i}\eta_\mathrm{f},2l\pm2\lambda+2,2l+2;x,y)=(1-y)^{-l-1+\mathrm{i}\eta_\mathrm{f}}$$
$$\times F_1(l\pm\lambda+1+\mathrm{i}\eta_\mathrm{i},l+1-\mathrm{i}\eta_\mathrm{f},l+1-\mathrm{i}\eta_\mathrm{f},2l\pm2\lambda+2;x,x/(1-y))$$
$$=(1-x-y)^{-l-1+\mathrm{i}\eta_\mathrm{f}}F_3(l\pm\lambda+1+\mathrm{i}\eta_\mathrm{i},l\pm\lambda+1-\mathrm{i}\eta_\mathrm{i},l+1$$
$$+\mathrm{i}\eta_\mathrm{f},l+1+\mathrm{i}\eta_\mathrm{f},2l+2;x,x^*)=\mathrm{e}^{\eta_\mathrm{f}\pi}(-x)^{-2l-2}\frac{(2l\pm2\lambda+1)!}{|\Gamma(l\pm\lambda+1+i\eta_\mathrm{i})|^2}(-1)^{l+1}$$
$$\times\Bigg\{2\mathbb{R}\frac{\Gamma(l\pm\lambda+1+\mathrm{i}\eta_\mathrm{i})\Gamma(-\lambda+\mathrm{i}\xi)}{\Gamma(l+1+\mathrm{i}\eta_\mathrm{f})}\left(-\frac{1}{x}\right)^{\lambda-\mathrm{i}\xi}F_2(-\lambda+1-\mathrm{i}\xi,l\pm\lambda+1$$
$$+\mathrm{i}\eta_\mathrm{i},l+1-\mathrm{i}\eta_\mathrm{f},\lambda+1-\mathrm{i}\xi,-\lambda+1-\mathrm{i}\xi;1/x,1/x^*)+\frac{|\Gamma(\lambda-\mathrm{i}\xi)|^2}{(2\lambda-1)!}$$
$$\times F_2(-2\lambda+1,l+1+\mathrm{i}\eta_\mathrm{f},l+1-\mathrm{i}\eta_\mathrm{f},-\lambda+1+\mathrm{i}\xi,-\lambda+1-\mathrm{i}\xi;1/x,1/x^*)\Bigg\}. \tag{11}$$

These Appell functions can be evaluated by the following convergent series [4, 8]:

$$F_1(\alpha,\beta,\beta',\gamma;x,y)=\sum\frac{(\alpha)_{m+n}(\beta)_m(\beta')_n}{(\gamma)_{m+n}m!n!}x^my^n\qquad\text{for } |x|<1 \text{ and } |y|<1 \tag{12}$$
$$F_2(\alpha,\beta,\beta',\gamma,\gamma';x,y)=\sum\frac{(\alpha)_{m+n}(\beta)_m(\beta')_n}{(\gamma)_m(\gamma')_nm!n!}x^my^n\qquad\text{for } |x|+|y|<1 \tag{13}$$
$$F_3(\alpha,\alpha',\beta,\beta',\gamma;x,y)=\sum\frac{(\alpha)_m(\alpha')_n(\beta)_m(\beta')_n}{(\gamma)_{m+n}m!n!}x^my^n\qquad\text{for } |x|<1 \text{ and } |y|<1 \tag{14}$$

where $(a)_n(=\Gamma(a+n)/\Gamma(a))$ is the Pochhammer symbol.

Our transformation (5) leads to the similar expression of $M_{l,l}^{-\lambda-1,q=0}$ derived by Alder *et al*. Applying equation (8) to (3), and then taking the limit of $l_\mathrm{i}=l_\mathrm{f}=l$ and $k_\mathrm{i}=k_\mathrm{f}=k$, we obtain the matrix elements:

$$M_{ll}^{-1,q}=\frac{|\Gamma(l+1+\mathrm{i}\eta)|^2}{(2l+1)!}\frac{1}{4k^2}\left(\frac{4k^2}{q^2+4k^2}\right)^{l+1}\mathrm{e}^{(2\theta-\pi)\eta}$$
$$\times{}_2F_1(l+1+\mathrm{i}\eta,l+1-\mathrm{i}\eta,2l+2;4k^2/(q^2+4k^2))\qquad\theta=\tan^{-1}(2k/q). \tag{15}$$

### 2.2. *General expression for* $|x| < 1 < |y|$ *or* $|y| < 1 < |x|$

Erdélyi [9] studied several generalized hypergeometric functions. He derived the relation between the Horn function $H_2$ and Appell function $F_2$ by means of these integral representations:

$$H_2(\alpha, \beta, \gamma, \delta, \epsilon; x, y) = \frac{\Gamma(1-\alpha)\Gamma(\delta-\gamma)}{\Gamma(1-\alpha-\gamma)\Gamma(\delta)} y^{-\gamma} F_2(\alpha+\gamma, \beta, \gamma, \epsilon, 1+\gamma-\delta; x, -1/y)$$
$$+\frac{\Gamma(1-\alpha)\Gamma(\gamma-\delta)}{\Gamma(1-\alpha-\delta)\Gamma(\gamma)} y^{-\delta} F_2(\alpha+\delta, \beta, \delta, \epsilon, 1+\delta-\gamma; x, -1/y). \quad (16)$$

This equation can be applied directly to the $F_2$ function in equation (3) if $|x| < 1 < |y|$ as follows:

$$F_2(l_\mathrm{i}+l_\mathrm{f}-\lambda+2, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, 2l_\mathrm{f}+2; x, y)$$
$$= (-1)^{l_\mathrm{f}-l_\mathrm{i}+\lambda} \frac{(2l_\mathrm{f}+1)!}{(l_\mathrm{i}+l_\mathrm{f}-\lambda+1)!} \left\{ \frac{\Gamma(-l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f})}{\Gamma(\lambda-l_\mathrm{i}-\mathrm{i}\eta_\mathrm{f})} (-y)^{-l_\mathrm{f}-1+\mathrm{i}\eta_\mathrm{f}} \right.$$
$$\times H_2(l_\mathrm{i}-\lambda+1+\mathrm{i}\eta_\mathrm{f}, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f}, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}; 2l_\mathrm{i}+2; x, -1/y)$$
$$-\frac{\Gamma(-l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f})(2l_\mathrm{f})!}{\Gamma(l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f})(\lambda-l_\mathrm{i}+l_\mathrm{f}-1)!} (-y)^{-2l_\mathrm{f}-1}$$
$$\left. \times F_2(l_\mathrm{i}-l_\mathrm{f}-\lambda+1, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}, -l_\mathrm{f}-\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, -2l_\mathrm{f}; x, y) \right\}. \quad (17)$$

When $|x| > 1 > |y|$, we can use the property of the $F_2$ function as follows:

$$F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y) = F_2(\alpha, \beta', \beta, \gamma', \gamma; y, x) \quad (18)$$

since the $F_2$ function is defined by equation (13). Finally we obtain the corresponding expression for $|x| > 1 > |y|$:

$$F_2(l_\mathrm{i}+l_\mathrm{f}-\lambda+2, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}, 2l_\mathrm{i}+2, 2l_\mathrm{f}+2; x, y)$$
$$= (-1)^{l_\mathrm{i}-l_\mathrm{f}+\lambda} \frac{(2l_\mathrm{i}+1)!}{(l_\mathrm{i}+l_\mathrm{f}-\lambda+1)!} \left\{ \frac{\Gamma(-l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i})}{\Gamma(\lambda-l_\mathrm{f}+\mathrm{i}\eta_\mathrm{i})} (-x)^{-l_\mathrm{i}-1-\mathrm{i}\eta_\mathrm{i}} \right.$$
$$\times H_2(l_\mathrm{f}-\lambda+1-\mathrm{i}\eta_\mathrm{i}, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}, -l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i}, l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i}; 2l_\mathrm{f}+2; y, -1/x)$$
$$-\frac{\Gamma(-l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i})(2l_\mathrm{i})!}{\Gamma(l_\mathrm{i}+1+\mathrm{i}\eta_\mathrm{i})(\lambda-l_\mathrm{f}+l_\mathrm{i}-1)!} (-x)^{-2l_\mathrm{i}-1}$$
$$\left. \times F_2(l_\mathrm{f}-l_\mathrm{i}-\lambda+1, l_\mathrm{f}+1-\mathrm{i}\eta_\mathrm{f}, -l_\mathrm{i}+\mathrm{i}\eta_\mathrm{i}, 2l_\mathrm{f}+2, -2l_\mathrm{i}; y, x) \right\}. \quad (19)$$

In these expressions (17) and (19), both $F_2$ functions in the right-hand side are reduced to polynomials, while the Horn function $H_2$ can be estimated directly by the expression:

$$H_2(\alpha, \beta, \gamma, \delta, \epsilon; x, y) = \sum_{\lambda=0}^{\infty} \sum_{u=0}^{\infty} \frac{(\alpha)_{\lambda-u}(\beta)_\lambda(\gamma)_u(\delta)_u}{(\epsilon)_\lambda \lambda! u!} x^\lambda y^u$$
$$= \sum_{k=0}^{\infty} \left\{ \sum_{n=0}^{[k/2]} \frac{(-1)^k(\beta)_n(\gamma)_{k-n}(\delta)_{k-n}}{(1-\alpha)_{k-2n}(\epsilon)_n n!(k-n)!} x^n y^{k-n} \right.$$
$$\left. + \sum_{n=[k/2]+1}^{k} \frac{(\alpha)_{2n-k}(\beta)_n(\gamma)_{k-n}(\delta)_{k-n}}{(\epsilon)_n n!(k-n)!} x^n y^{k-n} \right\} \quad (20)$$

where $[x]$ represents the largest integer less than $x$.

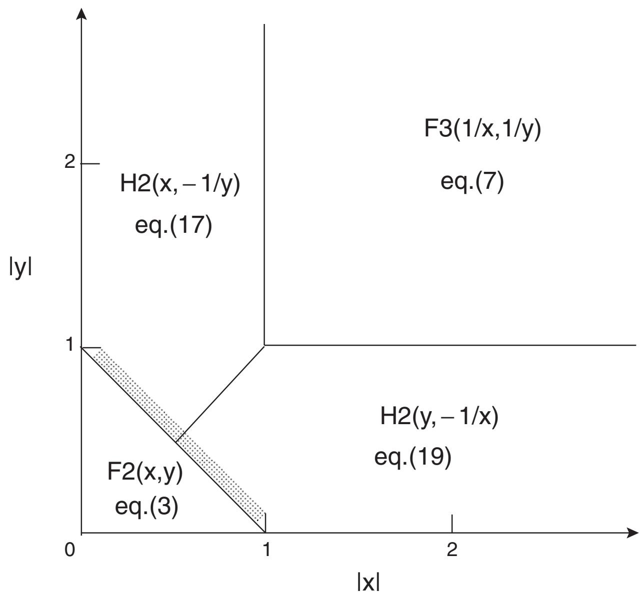


**Figure 1.** The schematic diagram of various expressions for $M_{l_\mathrm{i},l_\mathrm{f}}^{-\lambda-1,q}(x, y)$. The domain of convergence is shown by the symbols F2($F_2$), F3($F_3$) and H2($H_2$) with their relevant equations, respectively. The broad grey line gives an outline of the regions defined by $|1 - \mathbb{R}x|\sqrt{1 + (\mathbb{I}x)^2/(1 - \mathbb{R}x)^2} > |y| > |1 - \mathbb{R}x|$, and $|1 - \mathbb{R}y|\sqrt{1 + (\mathbb{I}y)^2/(1 - \mathbb{R}y)^2} > |x| > |1 - \mathbb{R}y|$, which corresponds to the exceptional regions where the integral expression (21) of Horn's function $H_2$ is not defined. For real variables $x$ and $y$, these regions become $|y| = |1 - x| > |x|$ and $|x| = |1 - y| > |y|$.

The integral representation of Horn's function $H_2(\alpha, \beta, \gamma, \delta, \epsilon; x', y')$ is given by Erdélyi [10] as follows:

$$\Gamma(\beta)\Gamma(\epsilon - \beta)H_2(\alpha, \beta, \gamma, \delta, \epsilon; x', y') = \Gamma(\epsilon)\int_0^1 u^{\beta-1}(1-u)^{\epsilon-\beta-1}(1-x'u)^{-\alpha}{}_2F_1(\gamma, \delta; 1-\alpha; -y'(1-x'u))\,\mathrm{d}u \quad (21)$$
$$0 < \mathbb{R}(\beta) < \mathbb{R}(\epsilon) \quad |x'| < 1 \quad |y'| < 1 \quad |1-x'||y'| < 1.$$

The variable ranges $|x'| < 1$, $|y'| < 1$ and $|1 - x'||y'| < 1$ lead to conditions such as $|y| > 1 > |x|$ and $|y| > |1 - x|$, or $|x| > 1 > |y|$ and $|x| > |1 - y|$ for equations (17) or (19), respectively. The schematic diagram for the convergent domain is shown in figure 1.

## 3. Application, results and conclusions

We apply our new formulae to obtain the radial matrix elements, which are necessary in the calculations for the electron-impact excitation of $O^{7+}$. The resulting values are compared with the corresponding numerical values, which are evaluated using Simpson's quadrature.

Figures 2 and 3 give the radial matrix elements of $O^{7+}$ for specific orbital angular momentum $l_\mathrm{i}$ and $l_\mathrm{f}$. The excitation energy of $O^{7+}$ (2s → 3p, 3d, or 2p → 3d) is 120.94 eV and the incident energy is given in these units (threshold units). Our revised formulae are very efficient in calculating the accurate matrix element, while Simpson's quadrature is time consuming since each Coulomb wave function is integrated over the radial coordinate up to 300 au with a relative accuracy less than $10^{-8}$ using the Adams' PECE method. Our analytic

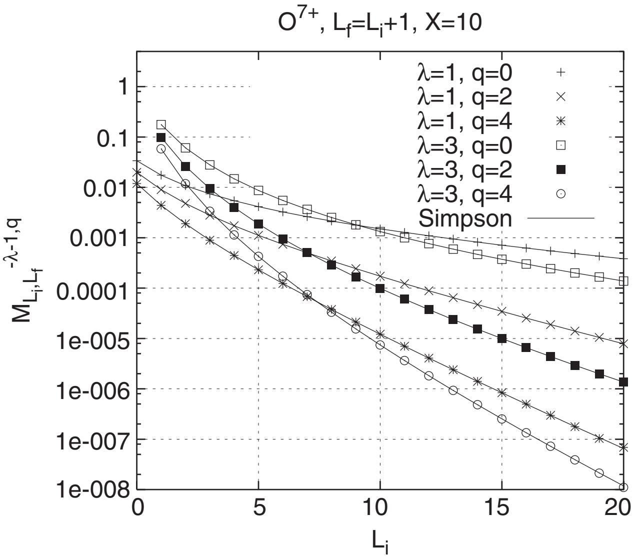


**Figure 2.** The radial matrix elements in electron–$O^{7+}$ (2s → 3p, 2s → 3d, 2p → 3d) scattering for $\lambda = 1$ and 3, $l_f = l_i + 1$, $q = 0$, 2 and 4, and the incident energy at $X = 10$ (threshold units) as a function of angular momentum $l_i$ calculated by our analytic formula (7). The full curves show the corresponding results of direct numerical integration (1) by Simpson's quadrature.

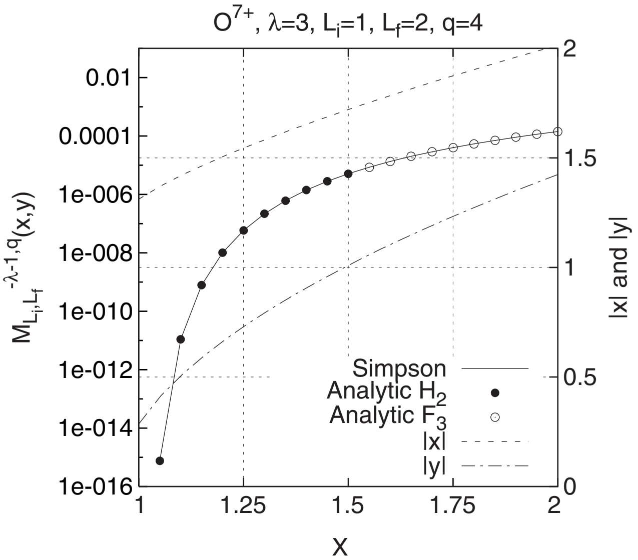


**Figure 3.** The radial matrix elements in electron–$O^{7+}$ (2s → 3p, 2s → 3d, 2p → 3d) scattering for $\lambda = 3$, $l_i = 1$, $l_f = 2$ and $q = 4$ as a function of incident energy $X$ (threshold units) calculated by our analytic formulae (7) and (19). The full curve shows the corresponding results of direct numerical integration (1) by Simpson's quadrature. The dotted curve and chaine curve show $|x|$ and $|y|$ defined by equation (4), respectively.

formula (7) is tested on our personal computer using the Fujitsu FORTRAN 95 compiler, and is 249 $\sim$ 5252 times faster than Simpson's quadrature with the Adams' PECE method for $\lambda = 3$, $l_{\rm i} = 0 \sim 5$, $l_{\rm f} = 0 \sim 5$, $q = 0 \sim 5$ and $3.56 < |y| < |x| < 38.98$. If one relaxes the convergence condition of the Adams' PECE method, such as the relative accuracies $10^{-4} \sim 10^{-5}$, the CPU time may be markedly decreased, while Simpson's quadrature does not reproduce the accurate matrix elements (7) for $l_{\rm i} > 4$ [11]. In figure 3, it is shown that our new formula (19) in terms of the Horn function works well for $|x| > 1 > |y|$.

We have pointed out that the most general expression of the radial Coulomb matrix element derived by Alder *et al* is erroneous and present accurate analytic expressions in terms of the generalized hypergeometric functions $F_3$ and $H_2$. These new formulae provide an effective method with respect to the evaluation of the transition matrix elements for multiple terms and higher partial waves because the convergent series (13) for $F_2$ works well whenever $|x| + |y| < 1$, while equation (7) can be used for $|x| > 1$ and $|y| > 1$, and then equation (17) or (19) may be applied when $|x| + |y| > 1$. The present formulae cover important regions for $|x|$ and $|y|$. Thus it is expected we will be able to calculate the radial Coulomb integral (1) analytically for various incident energies.

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