Recurrence relations for multipole radial integrals in the semiclassical Coulomb approximation

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It is shown that in the semiclassical (WKB) Coulomb approximation the radial integrals for multipole transitions in nonhydrogenic atoms obey simple recurrence relations. As a result, any such integral can be analytically expressed in terms of Anger functions plus an algebraic part proportional to $\sin\pi s$, where $s=\nu'-\nu$ is the difference between the effective principal quantum numbers of the states involved. We retrieve, in particular, various formulas established previously for dipole, quadrupole, and octupole transitions.

For many radiative transitions between Rydberg states, the semiclassical (WKB) form of the Coulomb approximation provides quite accurate results. Explicit analytical expressions in terms of Anger functions have been derived for dipole, quadrupole, and octupole radial matrix elements.[1–4] Here we show that these expressions obey simple recurrence relations similar to those known for the hydrogenic case.

In the semiclassical Coulomb approximation, the radial integral for a multipole transition of order L reads[1,5]

$$\mathcal{R}_L=\langle \nu l|r^L|\nu' l'\rangle =\frac{a^L}{\pi}\int_0^\pi du\,(1-\epsilon\cos u)^{L+1}\cos\psi \ , \tag{1}$$

where a is the Bohr radius, u is the eccentric anomaly, $\psi=su-s\epsilon\sin u-k\phi-(s-k)\pi$, $s=\nu'-\nu$, $k=l'-l$, and

$$\cos\phi=\frac{\cos u-\epsilon}{1-\epsilon\cos u} \ , \quad \sin\phi=\frac{(1-\epsilon^2)^{1/2}\sin u}{1-\epsilon\cos u} \ . \tag{2}$$

From Eq. (2) we obtain further

$$d\phi=\frac{(1-\epsilon^2)^{1/2}du}{1-\epsilon\cos u} \ . \tag{3}$$

By setting $u=\pi-\theta$, one can rewrite Eq. (1) in the form

$$\mathcal{R}_L=(-1)^k a^L I_{L+1,k}(s,\epsilon) \ , \tag{4}$$

where

$$I_{n,k}=\frac{1}{\pi}\int_0^\pi d\theta\,\tau^n\cos\psi_k \ , \tag{5}$$

and

$$\tau=1+\epsilon\cos\theta \ , \quad \chi=s(\theta+\epsilon\sin\theta) \ , \quad \psi_k=\chi+k\phi \ . \tag{6}$$

Notice that for $\theta=0$ one has $\phi=\pi$, $\chi=0$, while for $\theta=\pi$ one has $\phi=0$, $\chi=\pi s$. On the other hand, the differentials

$$d\tau=-\epsilon\sin\theta\,d\theta \ , \quad d\chi=s\tau\,d\theta \ , \quad \tau\,d\phi=-(1-\epsilon^2)^{1/2}d\theta \ , \tag{7}$$

readily follow from Eqs. (3) and (6).

Recurrence relations satisfied by the integrals $I_{n,k}$ are easily obtained on using the identity

$$\cos\psi_k=\cos\psi_{k\pm1}\cos\phi\pm\sin\psi_{k\pm1}\sin\phi \ . \tag{8}$$

Taking into account Eq. (7) and integrating by parts a few times one arrives at

$$I_{n+1,k}=aI_{n,k}+bI_{n,k-1}+c^{(-)}I_{n-1,k}+d \ , \tag{9a}$$

$$I_{n+1,k}=-aI_{n,k}-bI_{n,k+1}+c^{(+)}I_{n-1,k}+d \ , \tag{9b}$$

where [for brevity we put $\eta=(1-\epsilon^2)^{1/2}$]

$$a=n/s\eta \ , \quad b=n\epsilon/s\eta \ , \qquad c^{(\pm)}=(k\pm n)\eta/s \ , \quad d=(1-\epsilon)^n\frac{\sin\pi s}{\pi s} \ . \tag{10}$$

Notice that for $k=n$ one has $c^{(-)}=0$ in Eq. (9a), while $k=-n$ gives $c^{(+)}=0$ in Eq. (9b). Linear combinations of Eqs. (9a) and (9b) yield other interesting relations; for instance,

$$2I_{n,k}+\epsilon(I_{n,k+1}+I_{n,k-1})-2\eta^2 I_{n-1,k}=0\ . \tag{11}$$

To start the recurrence one can use

$$I_{0,0}=\mathbf{J}_s(-s\epsilon)\ ,\quad I_{1,0}=\frac{\sin\pi s}{\pi s}\ , \tag{12}$$

$$I_{1,\pm1}=\frac{\eta^2}{\epsilon}\mathbf{J}_s(-s\epsilon)\mp\eta\mathbf{J}_s'(-s\epsilon)-\frac{1}{\epsilon}\frac{\sin\pi s}{\pi s}\ , \tag{13}$$

where $\mathbf{J}_s(z)$ denotes the Anger function. From the integral representation of the latter,[6] one has indeed

$$\frac{1}{\pi}\int_0^\pi d\theta\cos\chi=\mathbf{J}_s(-s\epsilon)\ , \tag{14}$$

$$\frac{1}{\pi}\int_0^\pi d\theta\sin\chi\sin\theta=\mathbf{J}_s'(-s\epsilon)\ . \tag{15}$$

Accurate numerical values of the Anger functions may be obtained most conveniently from their rapidly convergent series expansions.

An obvious consequence of Eqs. (9)–(13) is that any integral $I_{n,k}$, and therefore $\mathcal{R}_L$, can be expressed in terms of $\mathbf{J}_s, \mathbf{J}_s'$, and an algebraical term times $(\sin\pi s)/\pi s$. A few specific cases are worked out below.

(i) Dipole transitions (L=1). Setting $n=1$, $k=1$ in Eq. (9a), $n=1$, $k=-1$ in Eq. (9b), and using Eqs. (12) and (13), one finds

$$\begin{aligned}I_{2,\pm1}&=\pm\frac{1}{s\eta}(I_{1,\pm1}+\epsilon I_{1,0})+(1-\epsilon)\frac{\sin\pi s}{\pi s}\\&=\pm\frac{\eta}{\epsilon s}\mathbf{J}_s-\frac{1}{s}\mathbf{J}_s'+\left[1-\epsilon\mp\frac{\eta}{\epsilon s}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{16}$$

Hence we recover the results established previously by Davydkin and Zon.[1] Similarly from Eq. (11) we obtain the auxiliary dipole function (forbidden by selection rules)

$$\begin{aligned}I_{2,0}&=-\frac{\epsilon}{2}(I_{2,1}+I_{2,-1})+\eta^2 I_{1,0}\\&=\frac{\epsilon}{s}\mathbf{J}_s'+(1-\epsilon)\frac{\sin\pi s}{\pi s}\ ,\end{aligned} \tag{17}$$

which will be needed below.

(ii) Quadrupole transitions (L=2). We set $n=2$, $k=0$, in both Eqs. (9a) and (9b), add the two expressions, and use Eq. (16) to get

$$\begin{aligned}I_{3,0}&=-\frac{\epsilon}{s\eta}(I_{2,1}-I_{2,-1})+(1-\epsilon)^2\frac{\sin\pi s}{\pi s}\\&=-\frac{2}{s^2}\mathbf{J}_s+\left[(1-\epsilon)^2+\frac{2}{s^2}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{18}$$

For $n=2$ taking $k=1$ in Eq. (9a) and $k=-1$ in Eq. (9b) in conjunction with Eqs. (13), (16), and (17), further give two auxiliary quadrupole functions:

$$\begin{aligned}I_{3,\pm1}&=\pm\frac{2}{s\eta}(I_{2,\pm1}+\epsilon I_{2,0})\mp\frac{\eta}{s}I_{1,\pm1}+(1-\epsilon)^2\frac{\sin\pi s}{\pi s}\\&=\left[\frac{2}{\epsilon s^2}\mp\frac{\eta^3}{\epsilon s}\right]\mathbf{J}_s+\left[\frac{\eta^2}{s}\mp\frac{2\eta}{s^2}\right]\mathbf{J}_s'\\&\quad+\left[(1-\epsilon)^2-\frac{2}{\epsilon s^2}\pm(2\epsilon+1)\frac{\eta}{\epsilon s}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{19}$$

Finally, for $n=3$, $k=\pm1$, Eq. (11) provides the radial integrals relevant for the case $l'-l=\pm2$:

$$\begin{aligned}I_{3,\pm2}&=-\frac{2}{\epsilon}I_{3,\pm1}-I_{3,0}+\frac{2\eta^2}{\epsilon}I_{2,\pm1}\\&=\left[\frac{2\epsilon^2-4}{\epsilon^2 s^2}\pm\frac{4\eta^3}{\epsilon^2 s}\right]\mathbf{J}_s+\left[\frac{4\epsilon^2-4}{\epsilon s}\pm\frac{4\eta}{\epsilon s^2}\right]\mathbf{J}_s'\\&\quad+\left[(1-\epsilon)^2+\frac{4-2\epsilon^2}{\epsilon^2 s^2}\pm2(\epsilon^2-2\epsilon-2)\frac{\eta}{\epsilon^2 s}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{20}$$

Equations (18) and (20) are in complete agreement with the formulas derived in Refs. 2 and 3.

(iii) Octupole transitions (L=3). We are now prepared to derive explicit expressions for octupole radial integrals. For instance, from Eqs. (9a) and (9b) we readily obtain for $n=3$, $k=\pm1$:

$$\begin{aligned}I_{4,\pm1}&=\mp\frac{3\epsilon}{2s\eta}(I_{3,\pm2}-I_{3,0})\pm\frac{\eta}{s}I_{2,\pm1}+(1-\epsilon)^3\frac{\sin\pi s}{\pi s}\\&=\left[\frac{6}{s^3}\mp\frac{5\eta}{s^2}\right]\left[\pm\frac{\eta}{\epsilon}\mathbf{J}_s-\mathbf{J}_s'\right]+\left[(1-\epsilon)^3-(2\epsilon^2-6\epsilon-5)\frac{1}{\epsilon s^2}\mp\left[\epsilon^2-\epsilon+\frac{6}{s^2}\right]\frac{\eta}{\epsilon s}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{21}$$

By using Eqs. (11), (18), and (21), we further get the auxiliary function

$$\begin{aligned}I_{4,0}&=-\frac{\epsilon}{2}(I_{4,1}+I_{4,-1})+\eta^2 I_{3,0}\\&=\frac{3\eta^2}{s^2}\mathbf{J}_s+\frac{6\epsilon}{s^3}\mathbf{J}_s'+\left[(1-\epsilon)^3-3(2\epsilon+1)\frac{1}{s^2}\right]\frac{\sin\pi s}{\pi s}\ .\end{aligned} \tag{22}$$

Equation (11) can be applied again to obtain

$$I_{4,\pm2}=-\frac{2}{\epsilon}I_{4,\pm1}-I_{4,0}+\frac{2\eta^2}{\epsilon}I_{3,\pm1}\ , \tag{23}$$

and

$$I_{4,\pm3}=-\frac{2}{\epsilon}I_{4,\pm2}-I_{4,\pm1}+\frac{2\eta^2}{\epsilon}I_{3,\pm2}\ . \tag{24}$$

Substitution of Eq. (23) into Eq. (24) finally gives for the radial integrals with $l'-l=\pm3$ the following result:

$$I_{4,\pm3}=\frac{4-\epsilon^2}{\epsilon^2}I_{4,\pm1}+\frac{2}{\epsilon}I_{4,0}+\frac{2\eta^2}{\epsilon}I_{3,\pm2}-\frac{4\eta^2}{\epsilon^2}I_{3,\pm1}$$

$$=\left[3(5\epsilon^2-12)\frac{\eta^2}{\epsilon^3 s^2}\pm6\left[\frac{2\eta^5}{\epsilon^3 s}+(4-\epsilon^2)\frac{\eta}{\epsilon^3 s^3}\right]\right]\mathbf{J}_s-\left[\frac{12\eta^4}{\epsilon^2 s}+6(4-3\epsilon^2)\frac{1}{\epsilon^2 s^3}\pm3(7\epsilon^2-12)\frac{\eta}{\epsilon^2 s^2}\right]\mathbf{J}'_s$$

$$+\left[(1-\epsilon)^3+(2\epsilon^4-6\epsilon^3-13\epsilon^2+8\epsilon+12)\frac{3}{\epsilon^3 s^2}\pm3\left[(1-\epsilon)(\epsilon^3-4\epsilon^2-8\epsilon-4)\frac{\eta}{\epsilon^3 s}+2(\epsilon^2-4)\frac{\eta}{\epsilon^3 s^3}\right]\right]\frac{\sin\pi s}{\pi s}\ . \qquad (25)$$

The expressions in Eqs. (21) and (25) have been derived recently by a direct calculation.[4] Needless to say, when s is a nonzero integer the sine terms in all the preceding formulas disappear and the Anger functions reduce to ordinary Bessel functions. It is easily checked that the simplified expressions so obtained for $L=1,2,3$ are equivalent to the hydrogenic results of Heim, Trautmann, and Baur.[5]

While it is obvious from Eq. (5) that $I_{n,k}(s,\epsilon)$ remains finite when $s\to0$, this limit is not readily worked out from the explicit analytic expressions derived above. The reason lies in the singularities of individual terms that must cancel before the final result is reached. Fortunately enough $I_{n,k}(0,\epsilon)$ can be calculated by straightforward integration for general n and k.[5] A simple alternative procedure is to start from

$$I_{n,0}(0,\epsilon)=\frac{1}{\pi}\int_0^\pi d\theta(1+\epsilon\cos\theta)^n=\eta^n P_n(1/\eta)\ , \qquad (26)$$

where P_n are the Legendre polynomials, and then use the recurrence relation

$$I_{n,k+1}(0,\epsilon)=\left[1+\frac{k}{n}\right]\frac{\eta^2}{\epsilon}I_{n-1,k}(0,\epsilon)-\frac{1}{\epsilon}I_{n,k}(0,\epsilon) \qquad (27)$$

obtained by multiplying Eq. (9b) by s and letting $s\to0$. This gives in particular

$$I_{n,\pm1}(0,\epsilon)=-(\epsilon/n)\eta^{n-1}P'_{n-1}(1/\eta) \qquad (28)$$

and

$$I_{n,\pm2}(0,\epsilon)=(1/n)\eta^{n-1}\{P'_n(1/\eta)-[(n+1)/(n-1)]\eta P'_{n-1}(1/\eta)\}\ . \qquad (29)$$

For low values $n=2-4$ one recovers in this way various special formulas relevant for the dipole, quadrupole, and octupole hydrogenic matrix elements given in Ref. 5.

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