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LETTER TO THE EDITOR

Fine and hyperfine structure parameters in a space of constant curvature

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Abstract. Analytical expressions of the atomic fine and hyperfine structure parameters in a space of constant curvature have been obtained by use of a ladder operator technique. It is found that the additional curvature contributions to the classical (flat) expressions increase with n.

In previous studies of atomic fine and hyperfine structure in a space of constant curvature, we have encountered integrals involving the 'pseudo-radial' part of the hydrogenic functions in a spherical three-space (Bessis and Bessis 1979, Bessis *et al* 1982, 1983; to be referred to as I, II and III, respectively). Indeed, the fine structure (Landé $\alpha_{\rm L}$ and spin curvature $\alpha_{\rm SC}$) and hyperfine structure (magnetic orbital, dipole–dipole and electric quadrupolar) parameters involve, respectively, the following integrals:

$$\alpha_{\rm L}=\left\langle nl\left|\frac{1}{R^3\sin^3\chi}\right|nl\right\rangle,\qquad \alpha_{\rm SC}=\left\langle nl\left|\frac{1-\cos\chi}{R^2\sin^2\chi}\right|nl\right\rangle,$$

$$\alpha_l=\left\langle nl\left|\frac{\cos\chi}{R^3\sin^3\chi}\right|nl\right\rangle,\qquad \alpha_{\rm d}=\left\langle nl\left|\frac{3-(1-\cos\chi)(2+\cos\chi)}{3R^3\sin^3\chi}\right|nl\right\rangle,\tag{1}$$

$$\alpha_{\rm Q}=\alpha_l,$$

where $|nl\rangle=(\sin\chi)^{-1}\mathcal{R}_{nl}(\chi)$ is the 'curved orbital', i.e. the eigenfunction of the hydrogenic Schrödinger equation in a space of constant positive curvature. In that space, the line and volume elements are

$$ds^2=R^2\,d\chi^2+R^2\sin^2\chi\,(d\theta^2+\sin^2\theta\,d\psi^2),\qquad d\tau=R^3\sin^2\chi\sin\theta\,d\chi\,d\theta\,d\psi,\tag{2}$$

where θ and ψ lie within their traditional bounds $0\leqslant\theta\leqslant\pi$ and $0\leqslant\psi\leqslant2\pi$.

Although χ is an angular variable ($0\leqslant\chi\leqslant\pi$), it can be related asymptotically to the 'flat' radial variable r ($0\leqslant r<\infty$). Indeed, at the asymptotic flat limit, as the curvature $1/R$ vanishes and $\chi\to0$ such that $R\chi=r$ remains finite, one finds again the ordinary (flat) results. In particular, the fine $\alpha_{\rm L}$ and hyperfine structure parameters α_l, $\alpha_{\rm d}$ and $\alpha_{\rm Q}$ converge towards the $\langle r^{-3}\rangle$ parameter while the spin curvature parameter $\alpha_{\rm SC}$ vanishes. The $\mathcal{R}_{nl}(\chi)$ functions are square integrable solutions of the eigenequation

$$\left(\frac{d^2}{d\chi^2}-\frac{l(l+1)}{\sin^2\chi}+2ZR\cot\chi+\lambda_n\right)\mathcal{R}_{nl}(\chi)=0.\tag{3}$$

They have been obtained in paper I.

$$\mathcal{R}_{nl}(\chi) = \mathcal{N}_{nl}(\sin\chi)^n \exp(-ZR\chi/n) P_v^{(\alpha,\beta)}(-\mathrm{i}\cot\chi) \tag{4}$$

where $\mathcal{N}_{nl}$ is the normalisation constant, $P_v^{(\alpha,\beta)}$ is a Jacobi polynomial of degree $v = n - l - 1$ with $\alpha = -n - \mathrm{i}ZR/n$ and $\beta = -n + \mathrm{i}ZR/n$; in spite of the presence of the imaginary quantities, it is a real polynomial in $\cot\chi$.

To our knowledge, integrals involving these functions are not yet available and their direct calculation, by termwise integration, leads to rather cumbersome expressions: only approximate expressions of α_{L} and α_{SC} for the particular case $l = n - 1$ and $l = n - 2$ have been derived in II.

In the present paper, a novel procedure of computation is proposed which leads to closed form expressions of the integrals (1) in terms of the n and l quantum numbers.

As pointed out in I, the eigenequation (3) is, within the Infeld and Hull (1951) classification, a type E (class I) factorisable equation. Therefore, the $\mathcal{R}_{nl}(\chi)$ functions are solutions of the following pair of difference differential equations:

$$\mathcal{H}_l^+\mathcal{R}_{nl-1} = (\lambda_n - L(l))^{1/2}\mathcal{R}_{nl}, \qquad \mathcal{H}_l^-\mathcal{R}_{nl} = (\lambda_n - L(l))^{1/2}\mathcal{R}_{nl-1}, \tag{5}$$

where the associated ladder operators $\mathcal{H}_l^\pm$, factorisation function $L(l)$ and eigenvalue λ_n are

$$\mathcal{H}_l^\pm = l\cot\chi - ZR/l \mp \mathrm{d}/\mathrm{d}\chi, \qquad L(l) = l^2 - Z^2R^2/l^2, \qquad \lambda_n = n^2 - Z^2R^2/n^2. \tag{6}$$

The present procedure takes advantage of equations (5) and (6) in the following way. Using the expressions of the ladder operators, one can write

$$\cot\chi = ZR/l^2 + (2l)^{-1}(\mathcal{H}_l^+ + \mathcal{H}_l^-) \tag{7a}$$

and/or

$$\cot\chi = ZR/(l-1)^2 + [2(l-1)]^{-1}(\mathcal{H}_{l-1}^+ + \mathcal{H}_{l-1}^-). \tag{7b}$$

Then, using equations (5) together with the mutual adjointness property of $\mathcal{H}_l^+$ and $\mathcal{H}_l^-$, one gets alternative expressions for the same matrix element involving any derivable function $F(\chi)$:

$$\begin{aligned}
&\langle nl-1|F\cot\chi|nl-1\rangle \\
&\quad = \frac{ZR}{l^2}\langle nl-1|F|nl-1\rangle - \frac{1}{2l}\left\langle nl-1\left|\frac{\mathrm{d}F}{\mathrm{d}\chi}\right|nl-1\right\rangle + \frac{\Lambda_n(l)}{l}\langle nl-1|F|nl\rangle \\
&\quad = \frac{ZR}{(l-1)^2}\langle nl-1|F|nl-1\rangle + \frac{1}{2(l-1)}\left\langle nl-1\left|\frac{\mathrm{d}F}{\mathrm{d}\chi}\right|nl-1\right\rangle \\
&\qquad + \frac{\Lambda_n(l-1)}{l-1}\langle nl-2|F|nl-1\rangle
\end{aligned} \tag{8}$$

where $\Lambda_n(l) = [\lambda_n - L(l)]^{1/2}$.

First, setting $F = 1$ in (8), one gets

$$\begin{aligned}
\langle nl-1|\cot\chi|nl-1\rangle &= \frac{ZR}{l^2} + \frac{\Lambda_n(l)}{l}\langle nl-1|nl\rangle \\
&= \frac{ZR}{(l-1)^2} + \frac{\Lambda_n(l-1)}{l-1}\langle nl-2|nl-1\rangle.
\end{aligned} \tag{9}$$

Therefore, this matrix element (9) must be independent of l and, since $\Lambda_n(n)=0$, it is equal to ZR/n^2. One gets, for any value of l,

$$\langle nl|\cot\chi|nl\rangle = ZR/n^2. \tag{10}$$

Setting in (8) $F=\cot\chi$, $F\cot\chi=(\sin^2\chi)^{-1}-1$ and using (10), one gets after some rearrangements

$$\begin{aligned}(l-1/2)\langle nl-1|(\sin^2\chi)^{-1}|nl-1\rangle \\ &= l+Z^2R^2/n^2l+\Lambda_n(l)\langle nl-1|\cot\chi|nl\rangle \\ &= (l-1)+Z^2R^2/n^2(l-1)+\Lambda_n(l-1)\langle nl-2|\cot\chi|nl-1\rangle.\end{aligned} \tag{11}$$

Using the same arguments as above, it follows that both right-hand sides of (11) are equal to $n+Z^2R^2/n^3$ and one gets

$$\langle nl|(\sin^2\chi)^{-1}|nl\rangle = Z^2R^2/(l+1/2)n^3+n/(l+1/2). \tag{12}$$

Setting $F=1/\sin^2\chi$ in (8), one gets

$$\begin{aligned}l(l-1)\langle nl-1|(\cos\chi)/\sin^3\chi|nl-1\rangle - ZR\langle nl-1|(\sin^2\chi)^{-1}|nl-1\rangle \\ &= l\Lambda_n(l)\langle nl-1|(\sin^2\chi)^{-1}|nl\rangle \\ &= (l-1)\Lambda_n(l-1)\langle nl-2|(\sin^2\chi)^{-1}|nl-1\rangle.\end{aligned} \tag{13}$$

Therefore, the combination (13) is independent of l and equal to zero. Using (12), one gets

$$\langle nl|(\cos\chi)/\sin^3\chi|nl\rangle = \frac{Z^3R^3}{n^3l(l+1)(l+1/2)}\left(1+\frac{n^4}{Z^2R^2}\right). \tag{14}$$

Now keeping in mind that, in the analysis of curvature effects, one is mainly interested in the predominant $1/R^2$ contributions, the asymptotic procedure described below is sufficient to yield the exact contribution required for the calculation (up to $1/R^2$) of the remaining integrals which are needed to derive analytical expressions of the parameters (1).

Let us note that, at the asymptotic flat limit, i.e. as $R\to\infty$, $\chi\to0$ such that $\chi R=r$, the curved hydrogenic function $\mathcal{R}_{nl}(\chi)$ converges to the classical one $R_{nl}(r)$ and therefore the integral $\langle nl|(2R\tan\frac{1}{2}\chi)^k|nl\rangle$ converges towards the flat hydrogenic integral $\langle r^k\rangle$. Then, after expanding the function in powers of $2R\tan\frac{1}{2}\chi$, one finds an approximate expression for the associated integral. In that way, one notes that

$$(1-\cos\chi)/R^2\sin^2\chi = \tfrac{1}{2}R^{-2}+\tfrac{1}{8}R^{-4}(2R\tan\tfrac{1}{2}\chi)^2$$

and one finds

$$\langle nl|(1-\cos\chi)/R^2\sin^2\chi|nl\rangle = (2R^2)^{-1}+\mathrm{O}(1/R^4). \tag{15}$$

Similarly, one notes that

$$\frac{1-\cos\chi}{R^3\sin^3\chi} = \frac{1}{2R^2}\left(\left(2R\tan\frac{\chi}{2}\right)^{-1}+\frac{1}{2R^2}\left(2R\tan\frac{\chi}{2}\right)+\frac{1}{16R^4}\left(2R\tan\frac{\chi}{2}\right)^3\right)$$

and, since $\langle r^{-1}\rangle = Z/n^2$, one finds

$$\langle nl|(1-\cos\chi)/R^3\sin^3\chi|nl\rangle = (2R^2)^{-1}Z/n^2+\mathrm{O}(1/R^4). \tag{16}$$

Finally, collecting the above results (10), (12), (14), (15) and (16), one obtains the following expressions for the parameters (1):

$$\begin{aligned} &\alpha_{\mathrm{L}} = \xi_{nl}\{1 + n[4n^3 + l(l+1)(2l+1)]/4Z^2R^2 + \mathrm{O}(1/R^4)\}, \\ &\alpha_{\mathrm{SC}} = 1/2R^2, \\ &\alpha_l = \alpha_{\mathrm{d}} = \alpha_{\mathrm{Q}} = \xi_{nl}[1 + n^4/Z^2R^2 + \mathrm{O}(1/R^4)], \end{aligned} \tag{17}$$

where $\xi_{nl} = \langle r^{-3}\rangle = Z^3/n^3 l(l+1)(l+1/2)$ is the well known flat limit expression of the parameters.

Although the hyperfine parameters show differentiated expressions (see equation (1)), nevertheless it follows from (17) that the $1/R^2$ contributions to those parameters are identical. As previously conjectured, the curvature effects increase with n.

Let us mention that the above procedure also provides, as a byproduct, off-diagonal (in l) matrix elements. For instance, following from equation (11), one gets

$$\Lambda_n(l)\langle nl-1|\cot\chi|nl\rangle = n - l + Z^2R^2/n^3 - Z^2R^2/n^2 l,$$

i.e.

$$\langle nl-1|\cot\chi|nl\rangle = -\frac{ZR}{n^2}\left(\frac{n-l}{n+l}\right)^{1/2}\left(1+\frac{n^2l^2}{Z^2R^2}\right)^{-1/2}\left(1-\frac{n^3 l}{Z^2R^2}\right). \tag{18}$$

Anticipating further investigation concerning atomic structure in the framework of a 'Dirac curved model', this procedure proves to be particularly valuable. Indeed, the two components of the 'curved Dirac' orbitals could be obtainable as a linear combination of curved generalised Kepler functions. In that case, since the quantum numbers are non integer, the calculation cannot be easily performed by a brute termwise integration.

This procedure, which has been suggested to us after reading a note of Lin (1941) concerning the normalisation of Dirac functions, can be applied to the calculation of matrix elements of Hermitian operators as long as the kets are solutions of a factorisable equation.

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