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1987 J. Phys. A: Math. Gen. 20 5745

(http://iopscience.iop.org/0305-4470/20/17/015)

J. Phys. A: Math. Gen. **20** (1987) 5745-5754. Printed in the UK

Algebraic recursive determination of matrix elements from ladder operator considerations

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Received 16 April 1987, in final form 19 June 1987

Abstract. A manufacturing process is proposed for calculating matrix elements of families of basic functions $Q_t(x)$ between the eigenfunctions $\Psi_j^m(x)$ of factorisable equations. This procedure, well adapted for computer algebra, relies on the well known property that solutions of factorisable equations are also solutions of a couple of first-order difference-differential equations. As a particular case, it is applied to the determination of closed form expressions of the 'curved' hydrogenic pseudoradial integrals which are needed when studying space-curvature effects in atomic structure calculations. Several other applications are pointed out.

1. Introduction

The computation of matrix elements $\langle j'm'|Q(x)|jm\rangle$ between solutions $\Psi_j^m(x)$ of factorisable equations is of particular interest in quantum physics. Indeed, in many cases, the wavefunctions are usually expanded on the basis of the eigenfunctions $\Psi_j^m(x)$ of model problems which usually lead, or are amenable to, the solution of factorisable equations. Without being exhaustive, let us recall that the associated spherical harmonics Y_l^m and generalised spherical harmonics $Y_{l,\gamma}^m$, the symmetric top functions $D_j^{mm'}$, the Gauss hypergeometric, Whittaker and Bessel functions, the harmonic oscillator, Morse oscillator, Pöschl-Teller, Manning-Rosen and Rosen-Morse diatomic vibration-rotation functions, the hydrogenic and generalised Kepler functions and many others are solutions of factorisable equations (Infeld and Hull 1951). Let us also mention that the Dirac radial functions in the usual Euclidean space (Infeld and Hull 1951) and also in a space of constant curvature can be expressed in terms of solutions of factorisable equations (Bessis *et al* 1984).

The concept of 'ladder operators' (for instance, the $J^{\pm}$ operators of angular momentum theory), being based on commutation rules and hermiticity, is a familiar one and operators of the form $K(x) \mp \mathrm{d}/\mathrm{d}x$ have also been used in simple approaches to supersymmetry (see, for instance, Killingbeck 1986). Let us briefly recall that, when a given equation is factorisable, one can take advantage of the existence of ladder operators $H_m^{\pm}$ acting on the eigenfunctions $\Psi_j^m(x)$ in order to obtain any $\langle j'm'|Q(x)|jm\rangle$ matrix elements in terms of the 'key' matrix elements $\langle j'j'|Q(x)|jj\rangle$ (Bessis *et al* 1973, 1975, Hadinger *et al* 1974). Nevertheless, this procedure, mainly using the ladder properties of the Ψ_j^m functions, may lead to somewhat cumbersome formulae involving

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0305-4470/87/175745+10$02.50

hardly reducible double summations, even for the case of diagonal ($j'=j$, $m'=m$) matrix elements. These summations may conceal a possibly simpler analytical dependence in the quantum numbers. On the other hand, one often has to calculate matrix elements of different $Q(x)$ operators which either can be directly regarded as belonging to a set of $Q_t(x)$ operators satisfying ladder relations or, alternatively, which can be expanded on such a basis Q_t. Although they were not explicitly demonstrated, such relations between the $Q_t(x)$ functions were underlying our previous techniques yielding closed form expressions of the fine and hyperfine structure parameters in a space of constant positive curvature (Bessis and Bessis 1983) and also of the Dirac-Coulomb radial r^l integrals (Bessis *et al* 1985).

In the present paper, it is shown that, when combining the different ladder relations satisfied both by the $\Psi_j^m(x)$ eigenfunctions and by a naturally adapted set of $Q_t(x)$ functions, one obtains algebraic formulae allowing an easy recursive computation of the $\langle j'm'|Q_t(x)|jm\rangle$ matrix elements between eigenfunctions of any factorisable equation (types A-F within the Infeld-Hull nomenclature).

After a necessary and brief recall of the factorisation scheme, the ladder properties to be satisfied by the $Q_t(x)$ functions are given and the associated algebraic recursive formulae relating the $\langle j'm'|Q_t(x)|jm\rangle$ matrix elements are derived. As an illustrative example, the determination of closed form expressions of the hydrogenic pseudoradial integrals $\langle nl|(\sin\chi)^l \exp(i\chi t)|nl\rangle$ and $\langle nl|(\sin\chi)^l \exp(i\chi t)|nl-1\rangle$ in a space of constant curvature is carried out. Indeed, the original motivation of setting up this technique was the need of analytical expressions of the curved-space parameters encountered when studying space-curvature effects in atomic structure calculations. Several other applications of the procedure are pointed out.

2. Factorisation scheme

After separating the variables, many model problems lead to the resolution of Sturm-Liouville differential equations which, by an adequate transformation of variable and function, can be always reduced to the standard form

$$(d^2/dx^2 + V(x,m) + \lambda_j)\Psi_j^m(x) = 0 \tag{1}$$

with associated boundary conditions ($x_1 \leqslant x \leqslant x_2$)

$$\Psi_j^m(x_1) = \Psi_j^m(x_2) = 0 \qquad \int_{x_1}^{x_2} |\Psi_j^m(x)|^2 \, dx = 1 \tag{2}$$

and where m is assumed to take successive discrete values labelling the eigenfunctions: $m = m_0, m_0+1, m_0+2, \ldots$.

Such an eigenequation (1) is factorisable when it can be replaced by each of the following two differential equations:

$$\begin{aligned} H_m^+ H_m^- \Psi_j^m &= (\lambda_j - L(m))\Psi_j^m \\ H_{m+1}^- H_{m+1}^+ \Psi_j^m &= (\lambda_j - L(m+1))\Psi_j^m \end{aligned} \tag{3}$$

where $H_m^\mp = K(x,m) \mp d/dx$ are the ladder operators; $K(x,m)$ and $L(m)$ are respectively the ladder and factorisation functions.

As stated by Schrödinger (1940b, 1941) and Infeld and Hull (1951), the eigenfunctions Ψ_j^m are then solutions of the following pair of difference-differential equations

$$\begin{aligned}(K(x,m)-\mathrm{d}/\mathrm{d}x)\Psi_j^{m-1}&=\Lambda_j(m)\Psi_j^m\\(K(x,m)+\mathrm{d}/\mathrm{d}x)\Psi_j^m&=\Lambda_j(m)\Psi_j^{m-1}\end{aligned}\tag{4}$$

where $\Lambda_j(m)=(\lambda_j-L(m))^{1/2}$.

These equations (4) allow the determination of any eigenfunction $\Psi_j^m(x)$, step by step, downward or upward, from the knowledge of any one of them and, particularly, from the knowledge of the 'key' eigenfunction which is the solution of a first-order differential equation.

For class I problems, i.e. when $L(m)$ is an increasing function of m, the eigenvalues are $\lambda_j=L(j+1)$. The necessary condition for the existence of quadratically integrable solutions, i.e. the quantisation condition is $j-m=v=\text{integer}\geqslant 0$. The 'key' eigenfunction ($v=0$) is a solution of the first-order differential equation

$$(K(x,j+1)-\mathrm{d}/\mathrm{d}x)\Psi_j^j(x)=0.\tag{5}$$

For class II problems, i.e. when $L(m)$ is a decreasing function of m, $\lambda_j=L(j)$, the quantisation condition is $m-j=v=\text{integer}\geqslant 0$ and the 'key' eigenfunction is a solution of the first-order differential equation

$$(K(x,j)+\mathrm{d}/\mathrm{d}x)\Psi_j^j(x)=0.\tag{6}$$

Infeld and Hull (1951) have found six fundamental factorisation types and have given the expressions of the $V(x,m)$ potential functions and associated ladder $K(x,m)$ and factorisation $L(m)$ functions allowing the factorisation of the eigenequation (1). Possible extensions to other potential functions exist via the 'artificial' or 'embedded' factorisation scheme (Schrödinger 1941, Infeld and Hull 1951) or also via the 'perturbed ladder operator method' (Bessis *et al* 1978, 1980, 1981, 1983). Let us now consider the calculation of matrix elements involving the $\Psi_j^m(x)$ functions.

3. Recursive determination of matrix elements

As far as one is concerned with the calculation of matrix elements, it seems quite natural to consider, at once, the ladder properties of the densities $(\Psi_{j'}^{m'}\Psi_j^m)$ rather than the individual ladder properties of the Ψ_j^m eigenfunctions themselves. Combining together (4) for Ψ_j^m and Ψ_j^{m-1} with their companions for $\Psi_{j'}^{m'}$ and $\Psi_{j'}^{m'-1}$, one can write

$$\begin{aligned}(\mathrm{d}/\mathrm{d}x)(\Psi_{j'}^{m'}\Psi_j^m)&=-(K+K')\Psi_{j'}^{m'}\Psi_j^m+\Lambda\Psi_{j'}^{m'}\Psi_j^{m-1}+\Lambda'\Psi_{j'}^{m'-1}\Psi_j^m\\(\mathrm{d}/\mathrm{d}x)(\Psi_{j'}^{m'-1}\Psi_j^{m-1})&=(K+K')\Psi_{j'}^{m'-1}\Psi_j^{m-1}-\Lambda\Psi_{j'}^{m'-1}\Psi_j^m-\Lambda'\Psi_{j'}^{m'}\Psi_j^{m-1}\\(\mathrm{d}/\mathrm{d}x)(\Psi_{j'}^{m'}\Psi_j^{m-1})&=(K-K')\Psi_{j'}^{m'}\Psi_j^{m-1}-\Lambda\Psi_{j'}^{m'}\Psi_j^m+\Lambda'\Psi_{j'}^{m'-1}\Psi_j^{m-1}\\(\mathrm{d}/\mathrm{d}x)(\Psi_{j'}^{m'-1}\Psi_j^m)&=-(K-K')\Psi_{j'}^{m'-1}\Psi_j^m+\Lambda\Psi_{j'}^{m'-1}\Psi_j^{m-1}-\Lambda'\Psi_{j'}^{m'}\Psi_j^m\end{aligned}\tag{7}$$

where the shortened notation $K=K(x,m)$, $K'=K(x,m')$, $\Lambda=\Lambda_j(m)$ and $\Lambda'=\Lambda_{j'}(m')$ is used.

When left-multiplying both sides of (7) by a sufficiently regular and derivable function $Q(x)$ on the interval (x_1,x_2), integrating by parts and taking into account the vanishing conditions (2) at the bounds, one obtains the following relations between

matrix elements involving the $Q(x)$ function, its derivative dQ/dx and the product $K(x, m)Q(x)$

$$\begin{aligned}
&\langle m'|\,dQ/dx-(K+K')Q\,|m\rangle+\Lambda\langle m'|\,Q\,|m-1\rangle+\Lambda\langle m'-1|\,Q\,|m\rangle=0\\
&\langle m'-1|\,dQ/dx+(K+K')Q\,|m-1\rangle-\Lambda\langle m'-1|\,Q\,|m\rangle-\Lambda'\langle m'|\,Q\,|m-1\rangle=0\\
&\langle m'|\,dQ/dx+(K-K')Q\,|m-1\rangle-\Lambda\langle m'|\,Q\,|m\rangle+\Lambda\langle m'-1|\,Q\,|m-1\rangle=0\\
&\langle m'-1|\,dQ/dx-(K-K')Q\,|m\rangle+\Lambda\langle m'-1|\,Q\,|m-1\rangle-\Lambda'\langle m'|\,Q\,|m\rangle=0
\end{aligned}\tag{8}$$

where $\langle m'|\,Q\,|m\rangle=\int_{x_1}^{x_2}\Psi_{j'}^{m'}\Psi_j^m Q(x)\,dx$.

When considering a suitable set of functions $Q_t(x)$ such that both the derivatives dQ_t/dx and the products $K(x, m)Q_t(x)$ can be written as finite expansions on the basis of the $Q_t(x)$ functions, the relations (8) can be easily transformed into algebraic recursive relations. Let us assume, for instance, that the following three-terms relations hold

$$\begin{aligned}
&K(x, m)Q_t(x)=a(t, m)Q_{t-1}+b(t, m)Q_t+c(t, m)Q_{t+1}\\
&dQ_t/dx=\alpha(t)Q_{t-1}+\beta(t)Q_t+\gamma(t)Q_{t+1}
\end{aligned}\tag{9}$$

and let us set

$$\begin{aligned}
&\mathfrak{X}_t=\int_{x_1}^{x_2}\Psi_{j'}^{m'}\Psi_j^m Q_t(x)\,dx \qquad \mathfrak{Y}_t=\int_{x_1}^{x_2}\Psi_{j'}^{m'}\Psi_j^{m-1}Q_t(x)\,dx\\
&\mathfrak{Z}_t=\int_{x_1}^{x_2}\Psi_{j'}^{m'-1}\Psi_j^{m-1}Q_t(x)\,dx \qquad \mathfrak{W}_t=\int_{x_1}^{x_2}\Psi_{j'}^{m'-1}\Psi_j^m Q_t(x)\,dx.
\end{aligned}\tag{10}$$

When building up a four-dimensional vector with the four integrals (10) and using (8) and (9), one obtains, in matrix notation, the following three-terms recurrence relation

$$\begin{vmatrix} A_1 & 0 & 0 & 0\\ 0 & A_2 & 0 & 0\\ 0 & 0 & A_3 & 0\\ 0 & 0 & 0 & A_4 \end{vmatrix}\begin{vmatrix} \mathfrak{X}_{t-1}\\ \mathfrak{Z}_{t-1}\\ \mathfrak{Y}_{t-1}\\ \mathfrak{W}_{t-1}\end{vmatrix}+\begin{vmatrix} B_1 & 0 & \Lambda & \Lambda'\\ 0 & B_2 & -\Lambda' & -\Lambda\\ -\Lambda & \Lambda' & B_3 & 0\\ -\Lambda' & \Lambda & 0 & B_4\end{vmatrix}\begin{vmatrix} \mathfrak{X}_t\\ \mathfrak{Z}_t\\ \mathfrak{Y}_t\\ \mathfrak{W}_t\end{vmatrix}$$
$$+\begin{vmatrix} C_1 & 0 & 0 & 0\\ 0 & C_2 & 0 & 0\\ 0 & 0 & C_3 & 0\\ 0 & 0 & 0 & C_4\end{vmatrix}\begin{vmatrix} \mathfrak{X}_{t+1}\\ \mathfrak{Z}_{t+1}\\ \mathfrak{Y}_{t+1}\\ \mathfrak{W}_{t+1}\end{vmatrix}=0 \tag{11}$$

where the following shortened notation is used: $A_1=\alpha-a-a'$, $A_2=\alpha+a+a'$, $A_3=\alpha+a-a'$, $A_4=\alpha-a+a'$, $B_1=\beta-b-b'$, $B_2=\beta+b+b'$, $B_3=\beta+b-b'$, $B_4=\beta-b+b'$, $C_1=\gamma-c-c'$, $C_2=\gamma+c+c'$, $C_3=\gamma+c-c'$, $C_4=\gamma-c+c'$, $a=a(t, m)$, $a'=a(t, m')$, $b=b(t, m)$, $b'=b(t, m')$, $c=c(t, m)$, $c'=c(t, m')$, $\alpha=\alpha(t)$, $\beta=\beta(t)$, $\gamma=\gamma(t)$, $\Lambda=(\lambda_j-L(m))^{1/2}$, $\Lambda'=(\lambda_{j'}-L(m'))^{1/2}$. Note that the j dependence of the matrices is entirely contained, via Λ and Λ', within the eigenvalue parameter λ_j.

Let us add that if (Q_t) is a suitable set of functions, the products $F_t(x)=g(x)Q_t(x)$ generate another suitable set (F_t) provided that $dg/g=k(x)\,dx$ where $k(x)$ has the same dependence in x as the ladder function $K(x, m)$. Of course, when applying the method to a given problem, one has to be careful in considering only $F_t(x)$ functions such that the product $F_t(x)\Psi_{j'}^{m'}(x)\Psi_j^m(x)$ still vanishes at the bounds x_1 and x_2.

The recurrence formula (11) is valid for all factorisation types and is well adapted for symbolic computation. It is, of course, quite useful for computing any $\langle j'm' | Q_t | jm \rangle$ matrix element as soon as matrix elements corresponding to a particular value $t = t_0$ are known. For several choices of the $Q_t(x)$ functions, formula (11), followed by few algebraic manipulations, allows the determination of closed-form expressions of the diagonal $\langle jm | Q_t | jm \rangle$ and of the subdiagonal $\langle jm | Q_t | jm-1 \rangle$ sets of integrals.

Obviously, an n-terms expansion (9) would lead to an n-terms recurrence relation between matrix elements (10). Not so infrequently, in many applications, one needs integrals (10) of families of functions $Q_t(x)$ leading to two-terms expansions (9) with $c(t, m) = \gamma(t) = 0$ (or $a(t, m) = \alpha(t) = 0$). Such is the case, for instance, of the hydrogenic $\langle r^t \rangle$ or, more generally, the $\langle r^t \exp(qr) \sin(pr) \rangle$ radial integrals, of the diatomic vibration-rotation $\langle r^t \rangle$ or $\langle r^t \exp(qr) \rangle$ and $\langle r^t \exp(qr) \cos(pr) \rangle$ nuclear integrals within the harmonic oscillator model (type D factorisation), of the $\langle \exp(-tr) \rangle$ or $\langle \exp(-tr + qe^r) \rangle$ nuclear integrals within the Morse-Pekeris model (type B factorisation) (see, for instance, Badawi *et al* 1973, 1974) and of several other models.

As a first illustrative example, we shall apply hereafter the recurrence relation (11) to the particular case of the $(j' = j, m' = m)$ integrals (10), denoted hereafter X_t, Y_t, Z_t and W_t, and consider $Q_t(x)$ functions leading to expansion formulae (9) with $c(t, m) = \gamma(t) = 0$. In that case, relations (11) reduce to $W_t = Y_t$ and

$$\begin{aligned} &(\alpha - 2a)X_{t-1} + (\beta - 2b)X_t + 2\Lambda Y_t = 0 \\ &(\alpha + 2a)Z_{t-1} + (\beta + 2b)Z_t - 2\Lambda Y_t = 0 \\ &\alpha Y_{t-1} + \beta Y_t - \Lambda X_t + \Lambda Z_t = 0 \end{aligned} \tag{12}$$

where the shortened notation $a = a(t, m)$, $\alpha = \alpha(t), \ldots,$ is used.

When $\beta \neq 0$, one obtains

$$\begin{vmatrix} X_t \\ Z_t \\ Y_t \end{vmatrix} = \Delta^{-1} \begin{vmatrix} 2\Lambda^2 + \beta(\beta+2b) & 2\Lambda^2 & -2\Lambda(\beta+2b) \\ 2\Lambda^2 & 2\Lambda^2 + \beta(\beta-2b) & 2\Lambda(\beta-2b) \\ \Lambda(\beta+2b) & -\Lambda(\beta-2b) & \beta^2 - 4b^2 \end{vmatrix} \begin{vmatrix} (\alpha-2a)X_{t-1} \\ (\alpha+2a)Z_{t-1} \\ \alpha Y_{t-1} \end{vmatrix} \tag{13}$$

where $\Delta = -\beta(4\Lambda^2 + \beta^2 - 4b^2)$.

When $\beta = 0$, the following three-terms recurrence relations are easily established:

$$\begin{aligned} &4\bar{\bar{\alpha}}(\Lambda^2 - \bar{b}\bar{\bar{b}})X_{t+1} - 2[\bar{\alpha}b(\bar{\bar{\alpha}} + 2\bar{\bar{a}}) - \bar{\bar{\alpha}}\bar{\bar{b}}(\bar{\alpha} - 2\bar{a})]X_t + (\bar{\bar{\alpha}} + 2\bar{\bar{a}})\bar{\alpha}(\alpha - 2a)X_{t-1} = 0 \\ &4(\Lambda^2 - \bar{b}\bar{\bar{b}})\bar{\alpha}\bar{\bar{\alpha}}Y_{t+1} - 4\bar{\alpha}\bar{b}(\bar{a}\bar{\bar{\alpha}} + \bar{\bar{a}}\bar{\alpha})Y_t + \alpha\bar{\alpha}(\bar{\alpha}^2 - 4\bar{a}^2)Y_{t-1} = 0 \end{aligned} \tag{14}$$

where, for convenience, the shortened notation $\alpha = \alpha(t)$, $\bar{\alpha} = \alpha(t+1)$, $\bar{\bar{\alpha}} = \alpha(t+2)$, $a = a(t, m)$, $\bar{a} = a(t+1, m), \ldots,$ is used.

Following the original motivation of this work, let us show how the above formulae can be used in order to obtain closed-form expressions of the hydrogenic pseudoradial integrals in a space of constant positive curvature. As already pointed out, the computation of these 'curved-space' integrals is not at all trivial, even though many of them correspond, at the asymptotic flat-space limit, to the familiar hydrogenic $\langle r^t \rangle$ radial integrals (Bessis and Bessis 1983, Bessis *et al* 1984).

4. Closed-form expressions of the 'curved-space' hydrogenic pseudoradial integrals

The interest building up a tractable 'curved-orbital' model (non-relativistic or relativistic) capable of exploring some space-curvature modifications of the atomic spectrum

has been outlined in a series of papers (Bessis and Bessis 1979, 1983, Bessis *et al* 1982, 1984, 1986). In that model, which, in many respects, may be considered as a preliminary step for further investigations of the gravitational modifications of the spectrum involving more elaborate curved spaces, the usual three-dimensional Euclidean flat space is simply substituted by a space of constant positive curvature, i.e. a three-dimensional hypersphere of radius R embedded in a four-dimensional Euclidean space. A direct parallel between 'curved-space' and 'flat-space' results is kept and, at the asymptotic flat-space limit, as $R \to \infty$, $\chi \to 0$ such that $R\chi = r$, the 'curved-space' solutions of quantum mechanical problems in hyperspherical coordinates (χ, θ, ϕ) converge towards the flat-space solutions in polar coordinates (r, θ, ϕ). Nevertheless, even for the case of one-electron atoms, closed-form expressions of many integrals are required in order to put in evidence the specific dependence of the space-curvature modifications of the spectrum in terms of the quantum numbers and are not still available.

After setting $\Phi_{nlM}(\chi, \theta, \phi) = (1/R \sin\chi)\Psi(\chi) Y_{lM}(\theta, \phi)$, the determination of the hydrogenic orbitals Φ_{nlM}, in a space of constant positive curvature, leads to the solution of the following Infeld–Hull type E (class I) factorisable equation (Schrödinger 1940a)

$$(\mathrm{d}^2/\mathrm{d}\chi^2 - m(m+1)/\sin^2\chi + 2ZR\cot\chi + \lambda_j)\Psi_j^m(\chi) = 0 \tag{15}$$

where $m = l$, $j = n-1$ and $\lambda_j = 2R^2E_n + 1$ is related to the electronic energy E_n.

The quantisation condition is $j - m = n - l - 1 = v = \text{integer} \geqslant 0$. The associated ladder and factorisation functions are

$$\begin{aligned} K(x, m) &= m\cot\chi - ZR/m \\ L(m) &= m^2 - Z^2R^2/m^2. \end{aligned} \tag{16}$$

For class I, $\lambda_j = L(j+1)$ and one obtains (in atomic units) $E_n = -Z^2/2n^2 + (n^2-1)/2R^2$.

From our previous studies, it can be inferred that, in fact, the determination of much of the integrals $\langle Q_t(\chi)\rangle$, which we need in atomic structure calculations, can be ultimately reduced to the evaluation of the integrals $\langle(\sin\chi)^t\cos(t\chi)\rangle$ and $\langle(\sin\chi)^t\sin(t\chi)\rangle$. This is the case, for instance, for the Coulombic interaction $\langle\cot\chi\rangle$, for the fine and hyperfine structure parameters (Bessis and Bessis 1983) and for many others involved in the interaction between atoms and external electromagnetic fields (Bessis *et al* 1986).

If one considers the set of the generating functions $Q_t(\chi) = (\sin\chi)^t \exp(-\mathrm{i}t\chi)$, it is easily checked that relations (9) are fulfilled with $a(t, m) = m$, $b(t, m) = -ZR/m - \mathrm{i}m$, $\alpha(t) = t$, $\beta(t) = -2\mathrm{i}t$ and $c(t, m) = \gamma(t) = 0$. Then, setting $t = 0$ in (12), after noting that $Q_0(\chi) = 1$ and that the eigenfunctions $\Psi_j^m(\chi)$ are assumed to be normalised, one obtains

$$\begin{aligned} X_0 &= Z_0 = 1 \\ X_{-1} &= Z_{-1} = (\Lambda_j(m)\, Y_0 - b(m))/a(m). \end{aligned} \tag{17}$$

Since the same expression (17) holds for $X_{-1} = \langle jm|Q_{-1}|jm\rangle$ and $Z_{-1} = \langle jm-1|Q_{-1}|jm-1\rangle$, it follows that this expression must be independent of m. Noting that for class I problems $\Lambda_j(j+1) = 0$, one obtains

$$\begin{aligned} X_{-1} &= Z_{-1} = -b(t, j+1)/a(t, j+1) \\ Y_0 &= (\Lambda_j(m))^{-1}(b(t, m) - a(t, m)b(t, j+1)/a(t, j+1)) \end{aligned} \tag{18}$$

and, after introducing the usual quantum numbers l and n, one obtains

$$\begin{aligned} \langle nl|\cot\chi|nl\rangle &= ZR/n^2 \\ \langle nl|nl-1\rangle &= ZRl\Lambda^{-1}(1/n^2 - 1/l^2) \end{aligned}$$

or alternatively

$$\langle nl\,|\,nl-1\rangle = -(l\Lambda/ZR)(1+n^2l^2/Z^2R^2)^{-1} \tag{19}$$

where

$$\Lambda = \Lambda_{nl} = (L(n)-L(l))^{1/2} = (ZR(n^2-l^2)^{1/2}/nl)(1+n^2l^2/Z^2R^2)^{1/2}. \tag{20}$$

Hence, using (13) together with the above expression of $Y_0 = \langle nl\,|\,nl-1\rangle$, one obtains

$$\begin{aligned} X_1 &= 4\Delta^{-1}\{n^2-1+l(l+1)+\mathrm{i}ZR[l(l+1)/n^2-3]\} \\ Z_1 &= 4\Delta^{-1}\{n^2-1+l(l-1)+\mathrm{i}ZR[l(l-1)/n^2-3]\} \\ Y_1 &= 4\Delta^{-1}\{(1/n^2-1/l^2)[ZRl(n^2+l^2-1)-\mathrm{i}l(3Z^2R^2+n^2l^2)]\} \end{aligned} \tag{21}$$

where $\Delta = 8[2ZR+\mathrm{i}(n^2-1-Z^2R^2/n^2)]$.

Since $\sin\chi\exp(-\mathrm{i}\chi) = \sin\chi\cos\chi - \mathrm{i}\sin^2\chi$, the separation of the real and imaginary parts in the expression (21) of X_1 and Y_1 easily yield the following expressions:

$$\begin{aligned} &\langle nl\,|\sin\chi\cos\chi\,|\,nl\rangle = \{3n^2-l(l+1)-(n^2/Z^2R^2)[n^4-n^2-l(l+1)(3n^2-1)]\}/2ZRD \\ &\langle nl\,|\sin^2\chi\,|\,nl\rangle = n^2\{5n^2+1-3l(l+1)-(n^2/Z^2R^2)(n^2-1)[n^2-1+l(l+l)]\}/2Z^2R^2D \\ &\langle nl\,|\sin\chi\cos\chi\,|\,nl-1\rangle = -n^2l\Lambda[3-n^2(n^2-1)/Z^2R^2]/2Z^2R^2D \\ &\langle nl\,|\sin^2\chi\,|\,nl-1\rangle = -n^2l\Lambda\{5n^2+1-l^2+(n^2/Z^2R^2) \\ &\qquad\times[n^4+n^2(3l^2-2)-l^2+1]\}/2Z^3R^3D' \end{aligned} \tag{22}$$

where $D = 1+2n^2(n^2+1)/Z^2R^2+n^4(n^2-1)^2/Z^4R^4$ and $D' = (1+n^2l^2/Z^2R^2)D$. Alternatively, after introducing into these expressions their flat-space limit and the additional space-curvature contributions (up to $1/R^2$) we obtain

$$\begin{aligned} &\langle nl\,|\,R\sin\chi\cos\chi\,|\,nl\rangle = \langle nl\,|\,r\,|\,nl\rangle - (n^2/2Z^3R^2)[7n^4+5n^2-l(l+1)(5n^2+1)] \\ &\langle nl\,|\,R^2\sin^2\chi\,|\,nl\rangle = \langle nl\,|\,r^2\,|\,nl\rangle - (n^2/2Z^4R^2)[11n^4-10n^2+3-l(l+1)(7n^2+5)] \\ &\langle nl\,|\,R^2\sin\chi\cos\chi\,|\,nl-1\rangle = \langle nl\,|\,r\,|\,nl-1\rangle - (n^4l\bar{\Lambda}/2Z^4R^2)(14n^2+10-3l^2) \\ &\langle nl\,|\,R^3\sin^2\chi\,|\,nl-1\rangle \\ &\qquad = \langle nl\,|\,r^2\,|\,nl-1\rangle + (n^4l\bar{\Lambda}/4Z^2R^2)[18n^4-14n^2(l^2-4)+(l^2-1)(l^2+2)] \end{aligned} \tag{23}$$

where $\bar{\Lambda}$ is the flat-space asymptotic limit of Λ.

The determination of analytical expressions of X_t and of Y_t can be pursued without difficulty, up to any higher positive value of t, by means of the relation (13) and one obtains, recursively, closed-form expressions of any curved-space integral $\langle nl\,|(\sin\chi)^t\cos(t\chi)\,|\,nl'\rangle$ or $\langle nl\,|(\sin\chi)^t\sin(t\chi)\,|\,nl'\rangle$ with $l'=l$ or $l'=l-1$.

For negative values of t, analytical expressions of X_t and Y_t are easily obtained by means of (12). Particularly, one again finds, in a straightforward way, our previous expressions of the fine and hyperfine structure parameters in a space of constant positive curvature which, at the asymptotic flat-space limit, all converge toward the classical $\langle r^{-3}\rangle$ parameters (Bessis and Bessis 1983). The determination of the curved-space integrals corresponding to lower negative values of t can be performed without any special difficulty. Selection rules follow from the vanishing conditions of the product $Q_t(\chi)\Psi_j^m\Psi_j^m$, or $Q_t(\chi)\Psi_j^m\Psi_j^{m-1}$, at the bounds 0 and π.

Note that closed-form expressions of the pseudoradial $\Psi_j^m(\chi)$ functions are known (Bessis and Bessis 1979), i.e.

$$\Psi_j^m(\chi) = N_{jm}(\sin\chi)^j \exp[-ZR\chi/(j+1)]P_v^{(w,w^*)}(-i\cot\chi) \tag{24}$$

where $w = -(j+1) - iZR/(j+1)$ and, in spite of the presence of the imaginary quantities, the Jacobi polynomial $P_v^{(w,w^*)}(\ )$ of degree $v = j - m = n - l - 1$ is a real polynomial in $\cot\chi$ and N_{jm} is a normalisation constant. Nevertheless, since w and w^* are non-integer, the computation of integrals such as (18) cannot be easily performed by a brute termwise integration.

Formulae (12) also work nicely to find again the closed-form expressions of the hydrogenic classical $\langle nl|r^t|nl\rangle$ and $\langle nl|r^t|nl-1\rangle$ radial integrals and to compute the radial integrals $\langle nl|r^t\exp(-qr)\sin(pr)|nl\rangle$, $\langle nl|r^t\exp(-qr)\cos(pr)|nl\rangle$, $\langle nl|r^t\exp(-qr)\sin(pr)|nl-1\rangle$ and $\langle nl|r^t\exp(-qr)\cos(pr)|nl-1\rangle$.

Indeed, the hydrogenic radial functions are $R_{nl}(r) = (1/r)\Psi_{nl}(r)$ where the $\Psi(r)$ functions are solutions of the type F (class I) factorisable equation

$$(d^2/dr^2 - m(m+1)/r^2 + 2Z/r + \bar{\lambda}_j)\Psi_j^m(r) = 0 \qquad 0 \leqslant r < \infty \tag{25}$$

where $m = l$, $j = n-1$ and $\bar{\lambda}_j = 2\bar{E}_n$.

The associated ladder and factorisation functions are $K(r, m) = m/r - Z/m$, $L(m) = -Z^2/m^2$ and, as a consequence, $\bar{\lambda}_j = L(j+1) = -Z^2/(j+1)^2$ and $\bar{E}_n = -Z^2/2n^2$.

It is easily checked that relations (9) are fulfilled by $Q_t(r) = r^t$ with $a(t, m) = m$, $b(t, m) = -Z/m$, $\alpha(t) = t$ and $\beta = c = \gamma = 0$. Relations (18) still hold for the flat-space integrals and again give the previously known expressions for $\langle 1/r\rangle$ and the overlap integral, respectively:

$$\begin{aligned} &\langle nl|1/r|nl\rangle = Z/n^2 \\ &\langle nl|nl-1\rangle = -Z\bar{\Lambda}_{nl}^{-1}(n^2-l^2)/n^2 l \end{aligned} \tag{26}$$

where $\bar{\Lambda}_{nl} = (L(n) - L(l)) = Z(n^2-l^2)^{1/2}/nl$. Since $\beta = 0$, one uses (14) and obtains the following recurrence formulae which, together with (26), allow the determination in closed form of the hydrogenic $\langle nl|r^t|nl\rangle$ and $\langle nl|r^t|nl-1\rangle$ integrals, for any value of t:

$$\begin{aligned} 4(t+2)Z^2\langle nl|r^{t+1}|nl\rangle &= 4Zn^2(2t+3)\langle nl|r^t|nl\rangle \\ &\quad - n^2(2l+t+2)(t+1)(2l-t)\langle nl|r^{t-1}|nl\rangle \\ 4(t+2)(t+1)Z^2\langle nl|r^{t+1}|nl-1\rangle &= 4Zn^2(2t+3)(t+1)\langle nl|r^t|nl-1\rangle \\ &\quad - n^2 t(t+2)(4l^2-(t+1)^2)\langle nl|r^{t-1}|nl-1\rangle. \end{aligned} \tag{27}$$

Of course, for this classical case, recurrence relations such as (27) are known for a long time (see, for instance, Durand 1970). They can also be obtained by means of hypervirial relations (see, for instance, Killingbeck 1978).

On the other hand, if one considers the set of generating functions $Q_t(r) = r^t\exp(-qr)$, where q is an arbitrary (real or complex) constant, relations (9) are fulfilled with $a(t, m) = m$, $b(t, m) = -Z/m$, $\alpha(t) = t$, $\beta(t) = -q$ and $c(t, m) = \gamma(t) = 0$. Hence, one can apply relation (13) in order to obtain the integrals X_t and Y_t in terms of X_0, Z_0 and $Y_0 = (\Lambda/\beta)(X_0 - Z_0)$ (see the last equation (12) for $t = 0$). Closed-form expressions of X_0 (and/or Z_0) are given by Gradshteyn and Ryzhik (1965).

Let us note that, for any derivable function $f(x)$, since $[\mathrm{d}/\mathrm{d}x, f] = \mathrm{d}f/\mathrm{d}x$, one easily obtains from (4) the following expression:

$$\langle jm|\mathrm{d}f/\mathrm{d}x|jm-1\rangle = \Lambda_j(m)(\langle jm|f(x)|jm\rangle - \langle jm-1|f(x)|jm-1\rangle). \tag{28}$$

In many cases, this expression can be used in order to obtain analytical expressions of the off-diagonal integrals $Y_t = \langle jm|Q_t|jm-1\rangle$.

For instance, it is easily checked that the curved-space hydrogenic integrals (22) satisfy the relation

$$\langle nl|\sin\chi\cos\chi|nl-1\rangle = \tfrac{1}{2}\Lambda_{nl}(\langle nl|\sin^2\chi|nl\rangle - \langle nl-1|\sin^2\chi|nl-1\rangle) \tag{29}$$

where Λ_{nl} is given in (19).

When dealing with the classical hydrogenic radial integrals, the following relation can be used:

$$\langle nl|r^t|nl-1\rangle = (t+1)^{-1}\bar{\Lambda}_{nl}(\langle nl|r^{t+1}|nl\rangle - \langle nl-1|r^{t+1}|nl-1\rangle) \tag{30}$$

where $\bar{\Lambda}_{nl}$ is given in (26).

5. Conclusion

Finally, it has been shown how one can establish recurrence formulae for computing matrix elements of $Q_t(x)$ functions between eigenfunctions $\Psi_j^m(x)$ of factorisable equations, as long as the $Q_t(x)$ functions satisfy relations such as (9). The procedure is valid for all types (A-F) of factorisation and is sufficiently versatile. Particularly, these recurrence formulae have allowed the determination of analytical expressions of the hydrogenic curved-space $\langle(\sin\chi)^t \exp(\mathrm{i}t\chi)\rangle$ integrals and flat-space $\langle r^t\rangle$ integrals without having to perform any quadrature. One part of the versatility of the technique comes from the fact that the choice of the $Q_t(x)$ functions is not unique. For instance, recurrence formulae (11) can be used for computing the curved-space $\langle(\sin\chi)^t \exp(q\chi)(\tan\chi)^t\rangle$ integrals ($a(t,m)=m$, $b(t,m)=ZR/m$, $\alpha(t)=t+p$, $\beta(t)=ZR$, $\gamma(t)=t$ and $c(t,m)=0$) or the $\langle(\sin\chi)^p \exp(q\chi)[\tan(\chi/2)]^t\rangle$ integrals ($a(t,m)=m/2$, $b(t,m)=ZR/m$, $c(t,m)=-m/2$, $\alpha(t)=(t+p)/2$, $\beta(t)=q$, and $\gamma(t)=(t-p)/2$).

It should be noted that formulae (11) may be useful not only for the E or F factorisation types but also in several other cases, such as for the computation of the type A $\langle[\tan(x/2)]^t\rangle$ integrals, the type B $\langle\exp(-tx)\rangle$ integrals, the type C or type D $\langle x^t\rangle$ integrals and, more generally, for the computation of the $\langle g(x)Q_t(x)\rangle$ integrals where $g(x)=(\sin x)^p[\tan(x/2)]^q$, $\exp(-px+q\,\mathrm{e}^x)$, $x^p\exp(qx^2)$ and $\exp(qx^2+px)$ for types A, B, C and D, respectively, and where p, q are arbitrary constants.

The eigenfunctions $\Psi_j^t(x)$ themselves can be considered as $Q_t(x)$ functions. Indeed, from (4), it is easily checked that they satisfy relations such as (9). For instance, for the case of the curved-space hydrogenic pseudoradial eigenfunctions, one obtains

$$\begin{aligned} K(\chi,m)\Psi_j^t &= [m/(2t+1)]\Lambda_j(t)\Psi_j^{t-1} + [ZR/m - ZRm/t(t+1)]\Psi_j^t \\ &\quad + [m/(2t+1)]\Lambda_j(t+1)\Psi_j^{t+1} \\ (\mathrm{d}/\mathrm{d}\chi)\Psi_j^t &= \tfrac{1}{2}[1-(2p-1)/(2t+1)]\Lambda_j(t)\Psi_j^{t-1} + [ZR(p-1)/t(t+1) - q])\Psi_j^t \\ &\quad - \tfrac{1}{2}[1+(2p-1)/(2t+1)]\Lambda_t(t+1)\Psi_j^{t+1}. \end{aligned} \tag{31}$$

The same relations hold for the flat-space hydrogenic radial functions $\Psi_j^t(r)$ (with Z in the place of ZR and the r variable in the place of the χ variable).

Let us remark that, since $\Lambda_t(t+1)=0$, the 'key' curved-space or the classical hydrogenic eigenfunctions Ψ_t^t satisfy two-terms expansions (9) with $c=\gamma=0$. This result holds for the other (B-D) factorisation types and class I or class II problems (for class I $\Lambda_t(t+1)=0$, $c=\gamma=0$ and for class II $\Lambda_t(t)=0$, $a=\alpha=0$). Nevertheless, an efficient application of the present technique to the determination of analytical expressions of the integrals over the product of three eigenfunctions of factorisable equations requires some more elaborate investigation. Computer programs which perform algebraic manipulations, such as REDUCE† or MACSYMA‡, would greatly help in that respect.

As a last remark, let us point out that formula (11) is still valid within all the extended factorisation schemes, i.e. when using the 'embedded' factorisation device or when using the perturbed ladder operator method. Indeed, in both cases, the 'embedded' eigenfunctions which depend on the artificial parameter or the 'perturbed' eigenfunctions are still solutions of a couple of first-order difference-differential equations (4) and vanish at the bounds (Infeld and Hull 1951, Bessis *et al* 1980, 1981, 1983). Nevertheless, within the perturbed ladder operator framework, the expression of the ladder function may become rather intricate and an adequate choice of $Q_t(x)$ functions leading to short finite expansions (9) may be more problematic.

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‡ MACSYMA, Reference Manual 1977 Laboratory of Computer Science, Massachusetts Institute of Technology, Cambridge, MA, USA.