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Algebraic recurrence formulae for matrix elements between the solutions of the transformed Jacobi eigenequation

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Abstract. The algebraic recursive determination of matrix elements of some selected families of functions $Q_t(x)$ between the solutions $\Psi_j^m(x)$ of factorisable equations is reinvestigated. The possibilities of the procedure outlined in a previous paper are enlarged by using the connection between factorisation types, i.e. the different possible factorisations of the same differential equation. The computation of matrix elements between the Jacobi eigenfunctions $\Psi_l^m(x) \simeq [\sin(ax/2)]^{\alpha+1/2}[\cos(ax/2)]^{\beta+1/2}P_v^{(\alpha,\beta)}(\cos ax)$, where a is a real or pure imaginary constant, is studied in detail. Algebraic recurrence formulae satisfied by matrix elements of $Q_t(x) = [\cos(ax/2)]^p[\sin(ax/2)]^q[\tan(ax/2)]^t$, $Q_t(x) = [\sin(ax)]^p[\tan(ax/2)]^q[\cos ax]^t$, $Q_t(x) = \Psi_l^t(x)$ and $Q_t(x) = \Psi_l^m(x)$ are given, and, for the particular cases $Q_t(x) = [\tan(ax/2)]^t$ and $Q_t(x) = (\cos ax)^t$, closed-form expressions are obtained. As an illustrative application, it is briefly shown how the expressions can serve to derive analytical approximations of the bound-state energies for the potential $V(x) = A\exp(-x^2) - l(l+1)/x^2$. Some further applications are pointed out.

1. Introduction

In a recent paper (Bessis and Bessis 1987, hereafter referred to as I), it has been shown how, when considering the different ladder relations satisfied both by the solutions $\Psi_j^m(x)$ of factorisable equations and by the naturally adapted set of $Q_t(x)$ functions, one obtains algebraic formulae which enable an easy recursive computation of the $\langle j'\, m'|Q_t(x)|j\, m\rangle$ matrix elements. In many cases, one 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 or, alternatively, can be expanded on such a basis $(Q_t(x))$. Such recurrence formulae may enable the determination of closed-form expressions for matrix elements of any $Q_t(x)$ as soon as those corresponding to some particular values of t are known. Particularly, closed-form expressions for the 'curved' hydrogenic pseudoradial integrals, which are needed when studying space curvature effects in atomic structure calculations, have been obtained without having to perform any quadrature.

As already pointed out in I, this algebraic procedure relies on the well known property that solutions of factorisable equations are also solutions of an equivalent couple of first-order difference-differential equations. It is valid for the six Infeld-Hull types of factorisation, denoted types A to F (Infeld and Hull 1951). In fact, these factorisation types are interrelated, i.e. by an adequate transformation of variable and function one can obtain an alternative factorisable equation corresponding to the same problem. Consequently the six factorisation types can be ultimately reduced to two fundamental types which, for convenience, can be denoted as 'trigonometric' types (types A and E) and as 'radial' types (types B, C, D and F). In this respect, the transformed Jacobi eigenequation, i.e. the type-A factorisable equation, can be regarded as the fundamental eigenequation for the trigonometric types and is of particular interest in computational physics: let us recall that, for instance, the associated spherical harmonics Y_L^M, the symmetric top functions or Wigner functions $D_{M,K}^{(L)}$, and more generally the Gauss hypergeometric functions, are simply related to the type-A eigenfunctions.

In the present paper, the algebraic recursive procedure is applied to the determination of type-A matrix elements. After a necessary and brief review of the factorisation scheme, it is shown how one can take advantage of the interconnection between types of factorisation to enlarge the range of applicability of our method (§ 2). Two different factorisations of the transformed Jacobi eigenequation are investigated and suitable sets of functions $Q_t(x)$ corresponding to each of these factorisations are proposed. Adequate families of $Q_t(x)$ functions, which can be used as an expansion basis for most $Q(x)$ of some interest are

$$Q_t(x)=[\cos(ax/2)]^p[\sin(ax/2)]^q[\tan(ax/2)]^t \qquad Q_t(x)=\Psi_j^l(x)$$

or

$$Q_t(x)=[\sin(ax)]^p[\tan(ax/2)]^q[\cos ax]^t \qquad Q_t(x)=\Psi_t^m(x)$$

where p and q are real arbitrary constants and, according to the boundary conditions of the physical problem under consideration, a is a real or a pure imaginary constant. The recurrence formulae satisfied by matrix elements of these $Q_t(x)$ functions are given and, for the particular cases $Q_t(x)=[\tan(ax/2)]^t$ and $Q_t(x)=(\cos ax)^t$, closed-form expressions are obtained (§ 3 and § 4). The above results, which are quite useful for computing integrals occurring in several quantum problems, may also be of interest for an analytical approximate treatment of non-factorisable eigenequations. As an illustrative example, it is briefly shown how, within the first-order perturbation scheme, fair analytical approximations to the bound-state energies for the potential $V(x)=A\exp(-x^2)-l(l+1)/x^2$ can be expressed in terms of the particular expressions ($a=1$ and $s=\frac{1}{5}$) of the $\langle j\,m|\ [\tan(ax/2)]^t|j\,m\rangle$ and $\langle j\,m|[\cos(ax/2)]^{-2s}[\tan(ax/2)]^t|j\,m\rangle$ matrix elements. Further possible applications are also considered in § 5.

2. The algebraic recursive procedure

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 reduce to the standard form

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

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

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

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

Let us assume that equation (1) is factorisable, i.e. that it can be replaced by each of the following two differential equations:

$$\begin{aligned} H_m^+ H_m^- \Psi_j^m &= (\lambda_j - L(m))^{1/2} \Psi_j^m(x) \\ H_{m+1}^- H_{m+1}^+ \Psi_j^m &= (\lambda_j - L(m+1))^{1/2} \Psi_j^m(x) \end{aligned} \tag{3}$$

where $L(m)$ does not depend on x and $H_m^\mp = K(x, m) \pm \mathrm{d}/\mathrm{d}x$ are ladder operators; $K(x, m)$ and $L(m)$ are respectively the ladder and factorisation functions.

As stated by Schrödinger (1940, 1941) and Infeld and Hull (1951), the eigenfunctions $\Psi_j^m(x)$ are then solutions of the following pair of first-order difference-differential equations:

$$\begin{aligned} (K(x, m) + \mathrm{d}/\mathrm{d}x)\Psi_j^m &= (\lambda_j - L(m))^{1/2} \Psi_j^{m-1} \\ (K(x, m) - \mathrm{d}/\mathrm{d}x)\Psi_j^{m-1} &= (\lambda_j - L(m))^{1/2} \Psi_j^m. \end{aligned} \tag{4}$$

The ladder operators $H_m^\mp$ generate the eigenfunctions, step by step, downward or upward, and allow the determination of any eigenfunction $\Psi_j^m(x)$ from the knowledge of any one of them and, particularly, from the knowledge of the 'key' eigenfunction $\Psi_j^j(x)$, which is solution of a first-order differential equation.

As has been shown in I, one can derive from the couple of first-order difference-differential equations (4) algebraic recursive formulae allowing the computation of matrix elements $\langle j'\, m'|Q_t(x)|j\, m\rangle$ between the $\Psi_j^m(x)$ functions, provided that both the derivative $\mathrm{d}Q_t/\mathrm{d}x$ and the product $K(x, m)Q_t(x)$ can be written as a short finite expansion on the basis of the $Q_t(x)$ functions. Of course, these conditions, to be fulfilled by the $Q_t(x)$ functions, restrict the range of applicability of the recursive procedure. It is therefore interesting to examine how the interrelation between factorisation types can be used so as to enlarge the field of matrix elements $\langle j'\, m'|Q_t(x)|j\, m\rangle$ obeying algebraic recurrence relations.

Let us consider the following transformation of variable and function:

$$x = u(\chi) \qquad \Psi(x) = C(f(x))^{1/2}\Phi(\chi) = C(F(\chi))^{1/2}\Phi(\chi) \tag{5}$$

where $C = C(j, m)$ is a normalisation conversion factor which is chosen in order to preserve the normalisation of the $\Psi_j^m(x)$ functions

$$\int_{x_1}^{x_2} |\Psi(x)|^2 \,\mathrm{d}x = C^2 \int_{\chi_1}^{\chi_2} |\Phi(\chi)|^2 F(\chi)(\mathrm{d}u/\mathrm{d}\chi)\,\mathrm{d}\chi = 1. \tag{6}$$

Let us assume that the change of the variable and function and the weight function $F(\chi)$ are chosen so that the factorisable equation (1) is transformed into another factorisable equation in the standard form

$$(\mathrm{d}^2/\mathrm{d}\chi^2 + V(\chi, M) + \lambda_J)\Phi_J^M(\chi) = 0. \tag{7}$$

Hence, the $\Phi_J^M(\chi)$ eigenfunctions are solutions of the difference-differential equations

$$\begin{aligned} (K(\chi, M) + \mathrm{d}/\mathrm{d}\chi)\Phi_J^M(\chi) &= (\lambda_J - L(M))^{1/2}\Phi_J^{M-1}(\chi) \\ (K(\chi, M) - \mathrm{d}/\mathrm{d}\chi)\Phi_J^{M-1}(\chi) &= (\lambda_J - L(M))^{1/2}\Phi_J^M(\chi) \end{aligned} \tag{8}$$

where $K(\chi, M)$ and $L(M)$ are the ladder and factorisation functions associated with the factorisable equation (7).

These equations (8) can be written again in terms of x and of the $\Psi(x)$ functions

$$\begin{aligned} (K_1(x) + f(x)\,\mathrm{d}/\mathrm{d}x)\Psi_1(x) &= \Lambda_1\Psi_2(x) \\ (K_2(x) - f(x)\,\mathrm{d}/\mathrm{d}x)\Psi_2(x) &= \Lambda_2\Psi_1(x) \end{aligned} \tag{9}$$

where Ψ_1 and Ψ_2 correspond to Φ_j^M and Φ_j^{M-1}, respectively; $K_1(x)=K_1(x,j,m)$ and $K_2=K_2(x,j,m)$ may depend on both quantum numbers j and m, and Λ_1, Λ_2 do not depend on x.

At this level, one can use quite the same considerations as in § 3 of I. Combining together (9) for Ψ_1 and Ψ_2 with their companions for Ψ_1' and Ψ_2', solutions of (9) with K_1', K_2', Λ_1' and Λ_2', one can write

$$\begin{aligned} f(x)\,\mathrm{d}(\Psi_1'\Psi_1)/\mathrm{d}x &= -(K_1+K_1')\Psi_1'\Psi_1+\Lambda_1\Psi_1'\Psi_2+\Lambda_1'\Psi_2'\Psi_1 \\ f(x)\,\mathrm{d}(\Psi_2'\Psi_2)/\mathrm{d}x &= (K_2+K_2')\Psi_2'\Psi_2-\Lambda_2\Psi_2'\Psi_1-\Lambda_2'\Psi_1'\Psi_2 \\ f(x)\,\mathrm{d}(\Psi_1'\Psi_2)/\mathrm{d}x &= (K_2-K_1')\Psi_1'\Psi_2-\Lambda_2\Psi_1'\Psi_1+\Lambda_1'\Psi_2'\Psi_2 \\ f(x)\,\mathrm{d}(\Psi_2'\Psi_1)/\mathrm{d}x &= -(K_1-K_2')\Psi_2'\Psi_1+\Lambda_1\Psi_2'\Psi_2-\Lambda_2'\Psi_1'\Psi_1 \end{aligned} \tag{10}$$

where the shortened notation $K_i'=K_i(x,j',m')$, $\Lambda_i'=\Lambda_i(j'm')$ is used.

When left-multiplying both sides of (10) by a sufficiently regular and differentiable 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, the derivative function $\mathrm{d}(fQ)/\mathrm{d}x$ and the products $K_1(x)Q(x)$ and $K_2(x)Q(x)$:

$$\begin{aligned} &\langle\Psi_1'|\,\mathrm{d}(fQ)/\mathrm{d}x-(K_1+K_1')Q|\Psi_1\rangle+\Lambda_1\langle\Psi_1'|Q|\Psi_2\rangle+\Lambda_1'\langle\Psi_2'|Q|\Psi_1\rangle=0 \\ &\langle\Psi_2'|\,\mathrm{d}(fQ)/\mathrm{d}x+(K_2+K_2')Q|\Psi_2\rangle-\Lambda_2\langle\Psi_2'|Q|\Psi_1\rangle-\Lambda_2'\langle\Psi_1'|Q|\Psi_2\rangle=0 \\ &\langle\Psi_1'|\,\mathrm{d}(fQ)/\mathrm{d}x+(K_2-K_1')Q|\Psi_2\rangle-\Lambda_2\langle\Psi_1'|Q|\Psi_1\rangle+\Lambda_1'\langle\Psi_2'|Q|\Psi_2\rangle=0 \\ &\langle\Psi_2'|\,\mathrm{d}(fQ)/\mathrm{d}x-(K_1-K_2')Q|\Psi_1\rangle+\Lambda_1\langle\Psi_2'|Q|\Psi_2\rangle-\Lambda_2'\langle\Psi_1'|Q|\Psi_1\rangle=0. \end{aligned} \tag{11}$$

Let us consider a suitable set of functions $Q_t(x)$ obeying, for instance, the following three-term relations:

$$\begin{aligned} \mathrm{d}(fQ_t)\,\mathrm{d}x &= a_0Q_{t-1}(x)+b_0Q_t(x)+c_0Q_{t+1}(x) \\ K_i(x)Q_t(x) &= a_iQ_{t-1}(x)+b_iQ_t(x)+c_iQ_{t+1}(x) \end{aligned} \tag{12}$$

where $i=1,2$, and let us set

$$\begin{aligned} \mathfrak{X}_t &= \int_{x_1}^{x_2}\Psi_1'(x)\Psi_1(x)Q_t(x)\,\mathrm{d}x \qquad & \mathfrak{Z}_t &= \int_{x_1}^{x_2}\Psi_2'(x)\Psi_2(x)Q_t(x)\,\mathrm{d}x \\ \mathfrak{Y}_t &= \int_{x_1}^{x_2}\Psi_1'(x)\Psi_2(x)Q_t(x)\,\mathrm{d}x \qquad & \mathfrak{W}_t &= \int_{x_1}^{x_2}\Psi_2'(x)\Psi_1(x)Q_t(x)\,\mathrm{d}x. \end{aligned} \tag{13}$$

From (11) and (12), one easily obtains, in matrix notation, the following three-term recurrence relation:

$$\begin{vmatrix} A_1 & 0 & 0 & 0 \\ 0 & A_2 & 0 & 0 \\ 0 & 0 & A_3 & 0 \\ 0 & 0 & 0 & A_4 \end{vmatrix}\begin{vmatrix} \mathfrak{X}_{t-1} \\ \mathfrak{Z}_{t-1} \\ \mathfrak{Y}_{t-1} \\ \mathfrak{W}_{t-1} \end{vmatrix} + \begin{vmatrix} B_1 & 0 & \Lambda_1 & \Lambda_1' \\ 0 & B_2 & -\Lambda_2' & -\Lambda_2 \\ -\Lambda_2 & \Lambda_1' & B_3 & 0 \\ -\Lambda_2' & \Lambda_1 & 0 & B_4 \end{vmatrix}\begin{vmatrix} \mathfrak{X}_t \\ \mathfrak{Z}_t \\ \mathfrak{Y}_t \\ \mathfrak{W}_t \end{vmatrix} + \begin{vmatrix} C_1 & 0 & 0 & 0 \\ 0 & C_2 & 0 & 0 \\ 0 & 0 & C_3 & 0 \\ 0 & 0 & 0 & C_4 \end{vmatrix}\begin{vmatrix} \mathfrak{X}_{t+1} \\ \mathfrak{Z}_{t+1} \\ \mathfrak{Y}_{t+1} \\ \mathfrak{W}_{t+1} \end{vmatrix} = 0. \tag{14}$$

where

$$A_1 = a_0 - a_1 - a'_1 \qquad A_2 = a_0 + a_2 + a'_2 \qquad A_3 = a_0 + a_2 - a'_1 \qquad A_4 = a_0 - a_1 + a'_2$$
$$B_1 = b_0 - b_1 - b'_1 \qquad B_2 = b_0 + b_2 + b'_2 \qquad B_3 = b_0 + b_2 - b'_1 \qquad B_4 = B_0 - b_1 + b'_2 \tag{15}$$
$$C_1 = c_0 - c_1 - c'_1 \qquad C_2 = c_0 + c_2 + c'_2 \qquad C_3 = c_0 + c_2 - c'_1 \qquad C_4 = c_0 - c_1 + c'_2.$$

Of course, when applying these relations to a given problem, one has to be careful in considering only $Q_t(x)$ functions such that the products $\Psi'_u(x)\Psi_s(x)Q_t(x)$ vanish at the bounds x_1 and x_2. An n-term expansion (12) would lead to an n-term recurrence relation between matrix elements (13).

When considering the particular case $\Psi'_1 = \Psi_1$, $\Psi'_2 = \Psi_2$, integrals (13) will be denoted X_t, Z_t, Y_t and W_t, and relations (14) reduce to $Y_t = W_t$ and

$$(a_0 - 2a_1)X_{t-1} + (b_0 - 2b_1)X_t + (c_0 - 2c_1)X_{t+1} + 2\Lambda_1 Y_t = 0$$
$$(a_0 + 2a_2)Z_{t-1} + (b_0 + 2b_2)Z_t + (c_0 + 2c_2)Z_{t+1} - 2\Lambda_2 Y_t = 0 \tag{16}$$
$$(a_0 + a_2 - a_1)Y_{t-1} + (b_0 + b_2 - b_1)Y_t + (c_0 + c_2 - c_1)Y_{t+1} - \Lambda_2 X_t + \Lambda_1 Z_t = 0.$$

Relations (14) and (16) are valid for all types of factorisation (A-F) and, as expected, when setting $f(x) = 1$, $\Psi_1 = \Psi_j^m$, $\Psi_2 = \Psi_j^{m-1}$, $\Psi'_1 = \Psi_{j'}^{m'}$ and $\Psi'_2 = \Psi_{j'}^{m'-1}$, one again finds relations (11) and (12) of I.

In the present paper we shall focus our attention on the determination of matrix elements between the Jacobi eigenfunctions, i.e. the general type-A matrix elements.

3. Type-A factorisation of the transformed Jacobi eigenequation

The transformed Jacobi eigenfunctions are solutions of the differential equation

$$\{\mathrm{d}^2/\mathrm{d}x^2 - a^2[m(m+1) + d^2 + 2d(m+\tfrac{1}{2})\cos ax]/\sin^2 ax + \lambda_j\}\Psi_j^m(x) = 0. \tag{17}$$

This equation is a type-A factorisable equation with associated ladder function $K(x, m)$ and factorisation function $L(m)$ (Infeld and Hull 1951)

$$K(x, m) = am \cot ax + ad/\sin ax \qquad L(m) = a^2m^2. \tag{18}$$

One has to distinguish two classes of factorisation (class I or class II) according to whether $L(m)$ is an increasing function of m (a is a real constant) or $L(m)$ is a decreasing function of m (a is a pure imaginary constant).

The necessary condition for the existence of a quadratically integrable solution of equation (17), i.e. the quantisation condition, is

$$\varepsilon(j - m) = v \tag{19}$$

where v is a positive integer and $\varepsilon = 1$ (or $\varepsilon = -1$) for class I (or class II) problems.

The associated eigenvalues are

$$\lambda_j = L(j + \varepsilon/2 + \tfrac{1}{2}). \tag{20}$$

Closed-form expressions of the eigenfunctions are known (Hadinger *et al* 1974)

$$\Psi_j^m(x) = N_{jm}[\sin(ax/2)]^{\alpha+1/2}[\cos(ax/2)]^{\beta+1/2}P_v^{(\alpha,\beta)}(\cos ax) \tag{21}$$

where N_{jm} is a normalisation constant, $P_v^{(\alpha,\beta)}(\,)$ is a Jacobi polynomial of degree v and

$$\alpha = \varepsilon(m + d + \tfrac{1}{2}) \qquad \beta = \varepsilon(m - d + \tfrac{1}{2}). \tag{22}$$

Since equation (17) is factorisable, the $\Psi_j^m(x)$ eigenfunctions are solutions of the first-order difference-differential equations (4), which are particular cases of the coupled equations (9), with $f(x)=1$, $\Psi_1(x)=\Psi_j^m(x)$, $\Psi_2(x)=\Psi_j^{m-1}(x)$, $K_1(x) = K_2(x)=K(x, m)$ and $\Lambda_1=\Lambda_2=(\lambda_j-L(m))^{1/2}$ and recurrence formulae for matrix elements of selected families of functions can be derived.

3.1. Recurrence formulae for the $\langle j\, m|g_1(x)\, [\tan(ax/2)]^t|j\, m\rangle$ matrix elements

In order to apply the algebraic recursive procedure, one has to consider suitable sets of functions $Q_t(x)$ obeying relations (12), i.e. such that both the derivative dQ_t/dx and the product $K(x, m)Q_t(x)$ can be written as finite expansions on the basis of the $Q_t(x)$ functions. Moreover, it is easily verified that, if $Q_t'(x)$ is a suitable set, the set of functions $Q_t(x)=g_1(x)Q_t'(x)$ is also a suitable set, provided that $dg_1/g_1=k_1(x)\,dx$, where $k_1(x)$ has the same x dependence as the ladder function $K(x, m)$.

Noting that the ladder function (18) can be written again $K(x, m)= [a(m+d)\cot(ax/2)]/2-[a(m-d)\tan(ax/2)]/2$, a suitable set is found to be

$$Q_t(x)=g_1(x)[\tan(ax/2)]^t \qquad g_1(x)=[\cos(ax/2)]^p[\sin(ax/2)]^q \tag{23}$$

where p and q are arbitrary (not necessarily integer) real constants.

Indeed, one gets the following two-term expansions:

$$\begin{aligned} dQ_t/dx &= [a(q+t)Q_{t-1}(x)-a(p-t)Q_{t+1}(x)]/2 \\ K(x, m)Q_t(x) &= [a(m+d)Q_{t-1}(x)-a(m-d)Q_{t+1}(x)]/2. \end{aligned} \tag{24}$$

Let us set

$$\begin{aligned} X_t(p, q) &= \langle j\, m|g_1(x)(\tan ax/2)^t|j\, m\rangle \\ Z_t(p, q) &= \langle j\, m-1|g_1(x)(\tan ax/2)^t|j\, m-1\rangle \\ Y_t(p, q) &= \langle j\, m-1|g_1(x)(\tan ax/2)^t|j\, m\rangle. \end{aligned} \tag{25}$$

From (24) it follows that matrix elements (25) obey relations (16) with

$$a_0=a(q+t)/2 \quad b_0=0 \quad c_0=-a(p-t)/2 \quad a_1=a_2=a(m+d)/2$$
$$b_1=b_2=0 \quad c_1=c_2=-a(m-d)/2$$

and one gets the following recurrence formulae:

$$\begin{aligned} &(t+q-2m-2d)X_{t-1}(\,)+(t-p+2m-2d)X_{t+1}(\,)+4\Lambda Y_t(\,)=0 \\ &(t+q+2m+2d)Z_{t-1}(\,)+(t-p-2m-2d)Z_{t+1}(\,)-4\Lambda Y_t(\,)=0 \\ &(t+q)Y_{t-1}(\,)+(t-p)Y_{t+1}(\,)-2\Lambda(X_t(\,)-Z_t(\,))=0 \end{aligned} \tag{26}$$

where $\Lambda=a^{-1}(\lambda_j-L(m))^{1/2}=(j+\varepsilon/2+\frac{1}{2}+m)^{1/2}(j+\varepsilon/2+\frac{1}{2}-m)^{1/2}$.

Note that the class dependence of the recurrence relations is entirely contained, through the binary class parameter ε ($\varepsilon=1$ or $\varepsilon=-1$ for class I or class II problems), in the expression of Λ.

As a particular case, when setting $p=q$ in the expressions (26), one obtains recurrence formulae for the determination of the $\langle j\, m|(\sin ax)^p[\tan(ax/2)]^t|j\, m\rangle$ matrix elements.

The above choice (23) of $Q_t(x)$ is not unique. For instance, the eigenfunctions $\Psi_j^t(x)$ themselves, and more generally, the $g_1(x)\Psi_j^t(x)$ functions, can also be considered as suitable $Q_t(x)$ functions. Indeed, from (4) and (18), one easily obtains the following three-term expansions:

$$\begin{aligned} \mathrm{d}\Psi_j^t/\mathrm{d}x &= [(t+\tfrac{3}{2})\Lambda_j(t)\Psi_j^{t-1} - 2ad\Psi_j^t - (t-\tfrac{1}{2})\Lambda_j(t+1)\Psi_j^{t+1}]/(2t+1) \\ K(x, m)\Psi_j^t(x) &= [m\Lambda_j(t)\Psi_j^{t-1} - 2ad(m+\tfrac{1}{2})\Psi_j^t + m\Lambda_t(t+1)\Psi_t^{t+1}]/(2t+1) \end{aligned} \tag{27}$$

where $\Lambda_j(t) = a(j+\varepsilon/2+\frac{1}{2}+t)^{1/2}(j+\varepsilon/2+\frac{1}{2}-t)^{1/2}$.

When dealing with problems leading to type-A (or perturbed type-A) eigenfunctions, an adequate expansion basis for the $Q(x)$ operators is known to be $Q_t(x) = [\tan(ax/2)]^t$. It is thus interesting to apply our method to the determination of closed-form expressions of matrix elements involving these functions.

3.2. Closed-form expressions for the $\langle j\, m|[\tan(ax/2)]^t|j\, m\rangle$ matrix elements

Let us set

$$\begin{aligned} X_t &= \langle j\, m|[\tan(ax/2)]^t|j\, m\rangle \\ Z_t &= \langle j\, m-1|[\tan(ax/2)]^t|j\, m-1\rangle \\ Y_t &= \langle j\, m-1|[\tan(ax/2)]^t|j\, m\rangle. \end{aligned} \tag{28}$$

Using relations (26) for the particular case $p = q = 0$, one gets the following relations between matrix elements (28):

$$\begin{aligned} &(t/2-m-d)X_{t-1} + (t/2+m-d)X_{t+1} + 2\Lambda Y_t = 0 \\ &(t/2+m+d)Z_{t-1} + (t/2-m+d)Z_{t+1} - 2\Lambda Y_t = 0 \\ &t(Y_{t-1} + Y_{t+1})/2 - \Lambda(X_t - Z_t) = 0. \end{aligned} \tag{29}$$

Substituting for Y_{t-1} and Y_{t+1} from the first equation (29) into the third equation yields

$$(m-d+t/2+\tfrac{1}{2})X_{t+2} = (2d-t)X_t - (4\Lambda^2/t)(X_t - Z_t) + (m+d-t/2+\tfrac{1}{2})X_{t-2}. \tag{30}$$

This relation enables the determination of X_{t+2} as soon as closed-form expressions for X_t (and therefore Z_t) and X_{t-2} are known. Since the $\Psi_j^m(x)$ eigenfunctions are assumed to be normalised: $X_0 = Z_0 = 1$; thus, in order to start the recursive process, one requires only a closed-form expression for X_2. The range of the x variable being different for class I and class II problems, the two cases have to be considered separately. In both cases, after a few algebraic manipulations, X_2 can be expressed in terms of normalisation integrals involving Jacobi polynomial and one obtains the following results (see appendix 1).

For class I problems (a is a real constant)

$$\langle j\, m|[\tan(ax/2)]^2|j\, m\rangle = -1 + 2(j+1)/(m-d+\tfrac{1}{2}). \tag{31}$$

For class II problems (a is a pure imaginary constant)

$$\langle j\, m|[\tanh(|a|x/2)]^2|j\, m\rangle = 1 - 2j/(m-d+\tfrac{1}{2}). \tag{32}$$

After introducing the binary class parameter ε, one obtains the unified expressionn

$$\varepsilon\, \langle j\, m|[\tan(ax/2)]^2|j\, m\rangle = -1 + 2(j+\varepsilon/2+\tfrac{1}{2})/(m-d+\tfrac{1}{2}). \tag{33}$$

Now, the recurrence relation (30) can be applied to calculate matrix elements (28). Using expression (33), one gets

$$X_2 - Z_2 = -2\varepsilon(j + \varepsilon/2 + \tfrac{1}{2})/(m - d - \tfrac{1}{2}). \tag{34}$$

Substituting for $(X_2 - Z_2)$ and X_2 from equations (33) and (34) in equation (30) and since $X_0 = 1$, one gets

$$\begin{aligned}\varepsilon\,\langle j\,m|[\tan(ax/2)]^4|j\,m\rangle &= 1 + 4(j + \varepsilon/2 + \tfrac{1}{2})[(d-1)/(m - d + \tfrac{3}{2})(m - d + \tfrac{1}{2})\\ &\quad + \Lambda^2/(m - d + \tfrac{3}{2})(m - d + \tfrac{1}{2})(m - d - \tfrac{1}{2})].\end{aligned} \tag{35}$$

Then, once X_2 and X_4 are known, one gets

$$\begin{aligned}\varepsilon\,\langle j\,m|[\tan(ax/2)]^6|j\,m\rangle &= -1 + 2(j + \varepsilon/2 + \tfrac{1}{2})[4(d-1)(d-2)/(m - d + \tfrac{1}{2})_3\\ &\quad + 4\Lambda^2(2d-3)/(m - d - \tfrac{1}{2})_4 + 6\Lambda^4/(m - d - \tfrac{3}{2})_5\\ &\quad + (m + d - \tfrac{3}{2})/(m - d + \tfrac{5}{2})(m - d + \tfrac{1}{2})]\end{aligned} \tag{36}$$

where $(u)_n = u(u+1)\ldots(u+n-1) = \Gamma(u+n)/\Gamma(u)$ is the Pochhammer symbol.

The determination of closed-form expressions for the $\langle j\,m|[\tan(ax/2)]^t|j\,m\rangle$ matrix elements can be pursued without special difficulty, up to any higher value of t, by means of relation (30).

Note that one can also apply the following four-term recurrence relation involving only the X_t:

$$\begin{aligned}(t+2)(m - d - t/2 - \tfrac{1}{2})(m - d + t/2 + \tfrac{3}{2})X_{t+4} &= [4(t+1)\Lambda^2 + t(m + d + t/2 + \tfrac{1}{2})(m - d + t/2 + \tfrac{1}{2})\\ &\quad + (t+2)(m - d - t/2 - \tfrac{1}{2})(2d - t - 2)]X_{t+2}\\ &\quad + [4(t+1)\Lambda^2 - t(m + d + t/2 + \tfrac{1}{2})(2d - t)\\ &\quad + (t+2)(m - d - t/2 - \tfrac{1}{2})(m + d - t/2 - \tfrac{1}{2})]X_t\\ &\quad - t(m + d + t/2 + \tfrac{1}{2})(m + d - t/2 + \tfrac{1}{2})X_{t-2}.\end{aligned} \tag{37}$$

This relation can be easily obtained from (29) after a few algebraic manipulations.

It should be mentioned that, without having to perform any integration, the above expressions for the $\varepsilon\,\langle j\,m|[\tan(ax/2)]^t|j\,m\rangle$ matrix elements have already been obtained, as a consequence of the expression of the first-order 'perturbed' factorisation function within the perturbed type-A ladder operator framework (Bessis and Bessis, unpublished).

Once closed-form expressions for the diagonal ($j' = j$, $m' = m$) matrix elements X_t have been obtained, the expressions of the subdiagonal ($j' = j$, $m' = m - 1$) matrix elements Y_t easily follow from (29):

$$Y_t = (2\Lambda)^{-1}[(d - t/2)(X_{t+1} + X_{t-1}) - m(X_{t+1} - X_{t-1})]. \tag{38}$$

It may happen that, for convergence considerations, an extended basis set, such as $Q_t(x) = [\cos(ax/2)]^{-2s}[\tan(ax/2)]^t$, constitutes a more convenient expansion basis for the operator $Q(x)$ under consideration and/or for the perturbed potentials. From (23), (26) and (16), it is easily found that matrix elements

$$X_t(s) = \langle j\,m|[\cos(ax/2)]^{-2s}[\tan(ax/2)]^t|j\,m\rangle$$

and $Z_t(s)$ obey the following recurrence relation:

$$(t-2s)(2m-2d-2s+t+1)X_{t+2}(s)$$
$$=[t(2d-t)-4s(m+d-t-\tfrac{1}{2})]X_t(s)-8\Lambda^2(X_t(s)$$
$$-Z_t(s))+t(2m+2d-t+1)X_{t-2}(s). \tag{39}$$

Now, in order to start the recursive procedure, one needs closed-form expressions for $X_0(s)$ and $X_2(s)$. Except the trivial case when s is an integer, the computation of these integrals involving s is somewhat more intricate than the computation of integral (33); nevertheless it can be shown that it is sufficient to evaluate $X_0(s)$, which can be still obtained from standard tables (Erdélyi *et al* 1954). One obtains (see appendix 1)

$$X_2(s)=X_0(s+1)-X_0(s)$$
$$X_0(s)=[2(j+1)\Gamma(v+s)\Gamma(m-d-s+\tfrac{3}{2})\Gamma(2j+2)]/$$
$$[v!\Gamma(m-d+\tfrac{1}{2})\Gamma(s)\Gamma(j+m-s+3)] \tag{40}$$
$$\times {}_4F_3(-v, j+m+2, m-d-s+\tfrac{3}{2}, 1-s; m-d+\tfrac{3}{2},$$
$$j+m-s+3, 1-v-s; 1)$$

where $v=\varepsilon(j-m)$ and ${}_4F_3(\ )$ is an hypergeometric function.

When considering only the above type-A factorisation of eigenequation (17), the possible choices of adequate $Q_t(x)$ functions, leading to short finite expansions such as (24) or (27), remains restricted. Let us enlarge the field of matrix elements $\langle j\, m|Q_t(x)|j\, m\rangle$ obeying algebraic recurrence relations by using the alternative (type-E) factorisation of eigenequation (17).

4. Type-E factorisation of the transformed Jacobi eigenequation

Let us consider the hyperbolic amplitude or Gudermannian transformation of variable and function connecting type-A and type-E factorisations and set

$$\tan(ax/2)=\exp(b\chi) \tag{41}$$
$$\Psi(x)=C(\sin ax)^{1/2}\Phi(\chi)=C(\cosh b\chi)^{-1/2}\Phi(\chi)$$

where $C=C(j, m)$ is a normalisation conversion factor (see equation (6)).

The transformed Jacobi eigenequation (17) can be rewritten

$$[\mathrm{d}^2/\mathrm{d}\chi^2+b^2(j+\varepsilon/2)(j+\varepsilon/2+1)/\cosh^2 b\chi+2b^2d(m+\tfrac{1}{2})\tanh b\chi+\lambda]\Phi(\chi)=0 \tag{42}$$

where $\lambda=-b^2[d^2+(m+\tfrac{1}{2})^2]$.

This last eigenequation can be identified with the standard Infeld–Hull type-E factorisable equation

$$[\mathrm{d}^2/\mathrm{d}\chi^2-A^2M(M+1)/\sin^2A(\chi+\chi_0)-2AQ\cot A(\chi+\chi_0)+\lambda_J]\Phi_J^M(\chi)=0 \tag{43}$$

where $A=\mathrm{i}b$, $\chi_0=\mathrm{i}\pi/2b$, $Q=-bd(m+\tfrac{1}{2})$, $J=m+\varepsilon/2$ and $M=j+\varepsilon/2$.

As a consequence, the associated quantisation condition is $J-M=m-j=v$, i.e. when $\Psi_j^m(x)$ is a solution of a type-A, class I ($\varepsilon=1$) problem (or a class II ($\varepsilon=-1$) problem), the corresponding eigenfunction $\Phi_J^M(\chi)$ is a solution of a type-E, class II (or class I) problem.

The associated ladder and factorisation functions are (Infeld and Hull 1951)

$$K(\chi, M) = AM \cot A(\chi+\chi_0) + Q/M \qquad L(M) = A^2M^2 - Q^2/M^2. \tag{44}$$

The associated ladder equations are

$$\begin{aligned}&[AM \cot A(\chi+\chi_0) + Q/M + \mathrm{d}/\mathrm{d}\chi]\Phi_J^M(\chi) = (\lambda_J - L(M))^{1/2}\Phi_J^{M-1}(\chi)\\ &[AM \cot A(\chi+\chi_0) + Q/M - \mathrm{d}/\mathrm{d}\chi]\Phi_J^{M-1}(\chi) = (\lambda_J - L(M))^{1/2}\Phi_J^M(\chi)\end{aligned} \tag{45}$$

where $(\lambda_J - L(M))^{1/2} = (L(J+\bar{\varepsilon}/2+\frac{1}{2}) - L(M))^{1/2}$ and $\bar{\varepsilon}$ is the type-E class parameter.

When returning to the original variable x and original eigenfunctions

$$\Psi_j^m(x) = C(j, m)(\cosh b\chi)^{-1/2}\Phi_J^M(\chi)$$

and

$$\Psi_{j-1}^m(x) = C(j-1, m)(\cosh b\chi)^{-1/2}\Phi_J^{M-1}(\chi),$$

the coupled equations (45) become

$$\begin{aligned}&(K_1(x, j, m) + a^{-1} \sin ax\, \mathrm{d}/\mathrm{d}x)\Psi_j^m(x) = \Lambda_1\Psi_{j-1}(x)\\ &(K_2(x, j, m) - a^{-1} \sin ax\, \mathrm{d}/\mathrm{d}x)\Psi_{j-1}^m(x) = \Lambda_2\Psi_j^m(x)\end{aligned} \tag{46}$$

where, in terms of the original type-A quantum numbers j, and m, and of the class parameter $\varepsilon = -\bar{\varepsilon}$

$$\begin{aligned}&K_1(x, j, m) = -(j+\varepsilon/2+\tfrac{1}{2}) \cos ax - d(m+\tfrac{1}{2})/(j+\varepsilon/2)\\ &K_2(x, j, m) = -(j+\varepsilon/2-\tfrac{1}{2}) \cos ax - d(m+\tfrac{1}{2})/(j+\varepsilon/2)\\ &\Lambda_1 = b^{-1}(\lambda_J - L(M))^{1/2}C(j, m)/(C(j-1, m)\\ &\Lambda_2 = b^{-1}(\lambda_J - L(M))^{1/2}C(j-1, m)/C(j, m).\end{aligned} \tag{47}$$

A closed-form expression for the normalisation conversion factor $C(j, m)$ can be obtained from ladder operator considerations (see appendix 2) and one gets

$$\begin{aligned}&\Lambda_1 = (j+\varepsilon/2+\tfrac{1}{2})\Delta \qquad \Lambda_2 = (j+\varepsilon/2-\tfrac{1}{2})\Delta\\ &\Delta = (j+\varepsilon/2)^{-1}[(j+\varepsilon/2-m-\tfrac{1}{2})(j+\varepsilon/2+m+\tfrac{1}{2})(j+\varepsilon/2-d)\\ &\qquad\times(j+\varepsilon/2+d)]^{1/2}[(j+\varepsilon/2-\tfrac{1}{2})(j+\varepsilon/2+\tfrac{1}{2})]^{-1/2}.\end{aligned} \tag{48}$$

Now, let us determine recurrence relations associated with the couple (46) of first-order difference-differential equations.

4.1. Recurrence formulae for the $\langle j\, m|g_2(x)(\cos ax)^t|j\, m\rangle$ matrix elements.

It is easily seen that suitable sets of $\bar{Q}_t(x)$ functions must satisfy relations (12) with the expressions (47) of $K_1(x) = K_1(x, j, m)$, $K_2(x) = K_2(x, j, m)$ and $f(x) = a^{-1} \sin ax$.

One particularly interesting set is found to be $\bar{Q}'_t(x) = (\cos ax)^t$ or, more generally,

$$\bar{Q}_t(x) = g_2(x)(\cos ax)^t \qquad g_2(x) = (\sin ax)^p(\tan ax/2)^q \tag{49}$$

where p and q are arbitrary (not necessarily integer) real constants.

Indeed, one gets the following three-term expansions:

$$\begin{aligned}&\mathrm{d}(a^{-1} \sin ax\bar{Q}_t)/\mathrm{d}x = -t\bar{Q}_{t-1} + q\bar{Q}_t + (p+t+1)\bar{Q}_{t+1}\\ &K_1(x)\bar{Q}_t(x) = -bd(m+\tfrac{1}{2})(j+\varepsilon/2)^{-1}\bar{Q}_t - b(j+\varepsilon/2+\tfrac{1}{2})\bar{Q}_{t+1}\\ &K_2(x)\bar{Q}_t(x) = -bd(m+\tfrac{1}{2})(j+\varepsilon/2)^{-1}\bar{Q}_t - b(j+\varepsilon/2-\tfrac{1}{2})\bar{Q}_{t+1}.\end{aligned} \tag{50}$$

Let us set

$$\bar{X}_t(p, q) = \langle j\, m|g_2(x)(\cos ax)^t|j\, m\rangle$$
$$\bar{Z}_t(p, q) = \langle j-1\ m|g_2(x)(\cos ax)^t|j-1\ m\rangle \tag{51}$$
$$\bar{Y}_t(p, q) = \langle j-1\ m|g_2(x)(\cos ax)^t|j\, m\rangle.$$

As a consequence of expansions (50), matrix elements (51) obey relations (16) with

$$a_0 = -t \qquad b_0 = q \qquad c_0 = p+t+1 \qquad a_1 = a_2 = 0$$
$$b_1 = b_2 = -d(m+\tfrac{1}{2})/(j+\varepsilon/2)$$
$$c_1 = -(j+\varepsilon/2+\tfrac{1}{2}) \quad c_2 = -(j+\varepsilon/2-\tfrac{1}{2})$$

and one gets

$$t\bar{X}_{t-1}(\ ) - [q+2d(m+\tfrac{1}{2})/(j+\varepsilon/2)]\bar{X}_t(\ )$$
$$-(2j+\varepsilon+p+t+2)\bar{X}_{t+1}(\ ) - 2\Lambda_1\bar{Y}_t(\ ) = 0$$
$$t\bar{Z}_{t-1}(\ ) - [q-2d(m+\tfrac{1}{2})/(j+\varepsilon/2)]\bar{Z}_t(\ )$$
$$+(2j+\varepsilon-p-t-2)\bar{X}_{t+1}(\ ) + 2\Lambda_2\bar{Y}_t(\ ) = 0 \tag{52}$$
$$t\bar{Y}_{t-1}(\ ) - q\bar{Y}_t(\ ) - (p+t+2)\bar{Y}_{t+1}(\ ) - \Lambda_1\bar{Z}_t(\ ) + \Lambda_2\bar{X}_t(\ ) = 0$$

where Λ_1 and Λ_2 are given by (48).

Let us now consider the determination of closed-form expressions for matrix elements.

4.2. Closed-form expressions for $\langle j\, m|(\cos ax)^t|j\, m\rangle$ matrix elements

Closed-form expressions for the $\langle j\, m|(\cos ax)^t|j\, m\rangle$ matrix elements can be obtained without having to perform any integration. Indeed, let us set

$$\bar{X}_t = \langle j\, m|(\cos ax)^t|j\, m\rangle$$
$$\bar{Z}_t = \langle j-1\ m|(\cos ax)^t|j-1,\ m\rangle \tag{53}$$
$$\bar{Y}_t = \langle j-1,\ m|(\cos ax)^t|j\, m\rangle.$$

For the particular case $p = q = 0$, relations (52) reduce to

$$t\bar{X}_{t-1} - [2d(m+\tfrac{1}{2})/(j+\varepsilon/2)]\bar{X}_t - (2j+\varepsilon+t+2)\bar{X}_{t+1} - 2\Lambda_1\bar{Y}_t = 0$$
$$t\bar{Z}_{t-1} + [2d(m+\tfrac{1}{2})/(j+\varepsilon/2)]\bar{Z}_t + (2j+\varepsilon-t-2)\bar{Z}_{t+1} + 2\Lambda_2\bar{Y}_t = 0 \tag{54}$$
$$t\bar{Y}_{t-1} - (t+2)\bar{Y}_{t+1} - \Lambda_1\bar{Z}_t + \Lambda_2\bar{X}_t = 0.$$

Since the eigenfunctions $\Psi_j^m(x)$ are orthonormalised, the particular values $\bar{X}_0 = \bar{Z}_0 = 1$ and $\bar{Y}_0 = 0$ are known. Setting $t = 0$ in the first and last equation (54), one gets the expressions of $\bar{X}_1$ and $\bar{Y}_1$, i.e.

$$\langle j\, m|\cos ax|j\, m\rangle = -d(m+\tfrac{1}{2})/(j+\varepsilon/2)(j+\varepsilon/2+1)$$
$$\langle j-1\ m|\cos ax|j,\ m\rangle = -\Delta/2 \tag{55}$$

where Δ is given by (48).

Then, setting $t=1$ in equation (54) and using (55), one gets the expressions for $\bar{X}_2$ and $\bar{Y}_2$, i.e.

$$\begin{aligned}\langle j\, m|(\cos ax)^2|j\, m\rangle &= [1+2d^2(m+\tfrac{1}{2})^2/(j+\varepsilon/2)^2(j+\varepsilon/2+1) \\ &\quad +(j+\varepsilon/2+\tfrac{1}{2})\Delta^2]/(2j+\varepsilon+3) \\ \langle j-1\, m|(\cos ax)^2|j\, m\rangle &= d(m+\tfrac{1}{2})\Delta/(j+\varepsilon/2-1)(j+\varepsilon/2+1).\end{aligned} \tag{56}$$

The determination of closed-form expressions for X_t and Y_t can be pursued without any special difficulty, up to any higher value of t.

Note that, since the Wigner functions $D^{(L)}_{M,M'}(\varphi, x, \psi)$ are simply related to the (class I) $\Psi^m_j(x)$ functions (see appendix 3), the expressions (55) (for $\varepsilon=1, j=L-\frac{1}{2}m=M-\frac{1}{2}$, and $d=M'$) again give the expansion coefficients of the product $(\cos x)D^{(L)}_{M,M'}(\phi, x, \psi)$ in terms of the $D^{(T)}_{M,M'}(\phi, x, \psi)$.

One can also obtain recurrence formulae (16) allowing the determination of the off-diagonal $\langle j-2\, m|(\cos ax)^t|j\, m\rangle$ matrix elements or, more generally of the $\langle j-k\, m|(\cos ax)^t|j\, m\rangle$, in terms of the diagonal elements. Indeed, it can be shown that $\Psi^m_{j-2}(x)$ and $\Psi^m_j(x)$ are solutions of coupled equations (9) and that the associated ladder conditions (12) are still satisfied by $(\cos ax)^t$. Applying equation (9) twice, where $f(x)$, $K_1(j)=K_1(x,j,m)$, $K_2(j)=K_2(x,j,m)$, $\Lambda_1=\Lambda_1(j)$ and $\Lambda_2=\Lambda_2(j)$ are given by (47) and (48), one gets

$$\begin{aligned}&(K_1(j-1)+f\,\mathrm{d}/\mathrm{d}x)(K_1(j)+f\,\mathrm{d}/\mathrm{d}x)\Psi^m_j(x)=\Lambda_1(j)\Lambda_1(j-1)\Psi^m_{j-2} \\ &\qquad (K_2(j)-f\mathrm{d}/\mathrm{d}x)(K_2(j-1)-f\,\mathrm{d}/\mathrm{d}x)\Psi^m_{j-2}(x)=\Lambda_2(j-1)\Lambda_2(j)\Psi^m_j.\end{aligned} \tag{57}$$

Keeping in mind that $\Psi^m_j(x)$ is solution of the second-order differential equation (17), one can write

$$(f^2\,\mathrm{d}^2/\mathrm{d}x^2)\Psi^m_j=[-(j+\varepsilon/2+\tfrac{1}{2})^2\sin^2 ax+m(m+1)+d^2+2d(m+\tfrac{1}{2})\cos ax]\Psi^m_j \tag{58}$$

and, consequently, it is easily found that $\Psi^m_j=\Psi_1$ and $\Psi^m_{j-2}=\Psi_2$ are solutions of the coupled equations (9) with

$$\begin{aligned}&f(x)=(\beta_0+\beta_1\cos ax)a^{-1}\sin ax \\ &K_1=\alpha_0+\alpha_1\cos ax+\alpha_2\cos^2 ax \qquad K_2=\alpha'_0+\alpha'_1\cos ax+\alpha'_2\cos^2 ax \\ &\Lambda_1=\Lambda_1(j)\Lambda_1(j-1) \qquad \Lambda_2=\Lambda_2(j)\Lambda_2(j-1) \\ &\alpha_0=m(m+1)+d^2-(j+\varepsilon/2+\tfrac{1}{2})(j+\varepsilon/2+\tfrac{3}{2})+d^2(m+\tfrac{1}{2})^2/(j+\varepsilon/2)(j+\varepsilon/2-1) \\ &\alpha_1=d(m+\tfrac{1}{2})[2+(j+\varepsilon/2+\tfrac{1}{2})/(j+\varepsilon/2-1)+(j+\varepsilon/2-\tfrac{1}{2})/(j+\varepsilon/2)] \\ &\alpha_2=2(j+\varepsilon/2+\tfrac{1}{2})^2 \\ &\beta_0=-\mathrm{d}(m+\tfrac{1}{2})(2j+\varepsilon-1)/(j+\varepsilon/2)(j+\varepsilon/2-1) \qquad \beta_1=-(2j+\varepsilon+1).\end{aligned} \tag{59}$$

It is easily checked that $(\cos ax)^t$ constitutes a suitable set of functions obeying the following four-term relations:

$$\begin{aligned}&\mathrm{d}[f(x)(\cos ax)^t]/\mathrm{d}x \\ &\quad =(-t\beta_0)(\cos ax)^{t-1}-(t+1)\beta_1(\cos ax)^t \\ &\qquad +(t+1)\beta_0(\cos ax)^{t+1}+(t+2)\beta_1(\cos ax)^{t+2} \\ &K_1(x)(\cos ax)^t=\alpha_0(\cos ax)^t+\alpha_1(\cos ax)^{t+1}+\alpha_2(\cos ax)^{t+2}\end{aligned} \tag{60}$$

and a straightforward generalisation of the first equation (16) yields

$$2\Lambda_1(j)\Lambda_1(j-1)\langle j-2\ m|(\cos ax)^t|j\ m\rangle$$
$$= -t\beta_0 X_{t-1} - [(t+1)\beta_1 + 2\alpha_0]X_t - [(t+1)\beta_0 - 2\alpha_1]X_{t+1}$$
$$-[(t+2)\beta_1 - 2\alpha_2]X_{t+2}. \qquad (61)$$

In the same way, applying equations (9) k times and using (57), one can obtain the coupled equations satisfied by Ψ^m_{j-k} and Ψ^m_j and, finally, the expression for the off-diagonal $\langle j-k\ m|(\cos ax)^t|j\ m\rangle$ matrix elements as a linear combination of the diagonal elements $\bar{X}_u = \langle j\ m|(\cos ax)^u|j\ m\rangle$.

As a last remark, let us add that the choice (49) of $Q_t(x)$ is not at all exhaustive. For instance, the $\Psi^m_t(x)$ functions themselves can be considered as $Q_t(x)$ functions. Indeed, from (46), it is easily found that they satisfy the expansions relations

$$\mathrm{d}(a^{-1}\sin ax\Psi^m_t)\,\mathrm{d}x = A_0\Psi^m_{t-1} + B_0\Psi^m_t + C_0\Psi^m_{t+1} \qquad (62)$$
$$K_i(x)\Psi^m_t = A_i\Psi^m_{t-1} + B_i\Psi^m_t + C_i\Psi^m_{t+1}$$

where

$$A_0 = (t+\varepsilon/2-\tfrac{1}{2})\Lambda_1(t)/(2t+\varepsilon+1) \qquad A_i = (j+\varepsilon/2\pm\tfrac{1}{2})\Lambda_1(t)/(2t+\varepsilon+1)$$
$$C_0 = (t+\varepsilon/2+\tfrac{3}{2})\Lambda_2(t+1)/(2t+\varepsilon+1) \qquad C_i = (j+\varepsilon/2\pm\tfrac{1}{2})\Lambda_2(t+1)/(2t+\varepsilon+1)$$
$$B_0 = -d(m+\tfrac{1}{2})/(t+\varepsilon/2)(2t+\varepsilon+1) \qquad B_i = 2d(m+\tfrac{1}{2})(j+\varepsilon/2\pm\tfrac{1}{2})/(t+\varepsilon/2)(2t+\varepsilon+1).$$

In the expressions for A_i, B_i and C_i, the upper and lower signs stand for $i=1$ and $i=2$, respectively.

5. Illustrative applications

If many real problems encountered in physics, or even many (sufficiently elaborated) model problems, do not lead to the solution of factorisable equations, nevertheless, in most cases of interest, they can be conveniently described by a kernel potential belonging to one of the factorisable types together with an additional perturbation term. Maybe, not at all fortuitously, well adapted expansion bases for the perturbation turn out to be suitable sets of $Q_t(x)$ functions: when dealing with type-A unperturbed problems, such is the case, for instance, for $Q_t(x) = [\tan(ax/2)]^t$ or $Q_t(x) = (\cos ax)^t$.

As an illustrative application, let us determine analytical approximations to the bound-state energies of the Schrödinger equation with a radial Gaussian potential (for an accurate treatment, see Buck (1977), Stephenson (1977) or Lai (1983) and references therein)

$$(\mathrm{d}^2/\mathrm{d}x^2 + A\exp(-x^2) - l(l+1)/x^2 + E)\Psi(x) = 0 \qquad (63)$$

with the associated boundary conditions $\Psi(0) = \Psi(\infty) = 0$.

As already pointed out (Bessis *et al* 1982), good analytical approximations to the energies can be obtained by means of the traditional Rayleigh–Schrödinger method. Noting that the Gaussian potential $\exp(-x^2)$ behaves as $(\cosh x)^{-2}$ and the rotational term x^{-2} resembles $(\sinh x)^{-2}$, a suitable and exactly soluble unperturbed wave equation is

$$[\mathrm{d}^2/\mathrm{d}x^2 + A/(\cosh x)^2 - l(l+1)/(\sinh x)^2 + E^{(0)}]\Psi^{(0)}(x) = 0. \qquad (64)$$

Setting $A=\mu^2-\frac{1}{4}$, $m=-(l+\mu+\frac{3}{2})/2$, $d=(\mu-l-\frac{1}{2})/2$, this equation (64) can re-written as

$$\{d^2/dx^2+4[m(m+1)+d^2+2d(m+\tfrac{1}{2})\cosh 2x]/(\sinh 2x)^2+E^{(0)}\}\Psi_{jm}^{(0)}=0. \quad (65)$$

This is a factorisable type-A (class II) eigenequation (17) with $a=2i$, $L(m)=-4m^2$; the associated quantisation condition is $m-j=n=\text{integer}\geq 0$. In order to satisfy the boundary conditions, the condition $\mu\leq-(n+l+1)$ must hold and one has to choose the negative solution of $\mu^2-\frac{1}{4}=A$, i.e. $\mu=-(A+\frac{1}{4})^{1/2}$.

The perturbed bound-state energies are

$$E^{(0)}=-L(j)=-(2n+l+\mu+\tfrac{3}{2})^2 \quad (66)$$

The perturbation to be considered is

$$V(x)=A[\exp(-x^2)-(\cosh x)^{-2}]-l(l+1)[x^{-2}-(\sinh x)^{-2}]. \quad (67)$$

A direct computation of matrix elements of $V(x)$ on the basis of the eigenfunctions $\Psi_{jm}^{(0)}$ is not all easy to perform. Therefore, it is convenient to consider the following expansions:

$$\begin{aligned}\exp(-x^2)-(\cosh x)^{-2}&=\sum_{t=2}a_t(\tanh x)^{2t}\\ x^{-2}-(\sinh x)^{-2}&=\tfrac{1}{3}(\cosh x)^{-2/5}+\sum_{t=2}b_t(\tanh x)^{2t}\end{aligned} \quad (68)$$

where the first term in the second equation of (68) has been found by noting that $x^{-2}-(\sinh x)^{-2}=\frac{1}{3}-x^2/15+\ldots$ and that $(\cosh x)^{-2/5}=1-x^2/5+\ldots$.

Finally the perturbation can be rewritten as

$$V(x)=l(l+1)(\cosh x)^{-2/5}/3+\sum_{t=2}[Aa_t-l(l+1)b_t](\tanh x)^{2t}. \quad (69)$$

And, within the Rayleigh-Schrodinger framework, the first-order perturbed energy is

$$E_{jm}^{(1)}=-(2n+l+\mu+\tfrac{3}{2})^2+l(l+1)X_0(s=\tfrac{1}{5})/3+\sum_{t=2}[Aa_t-l(l+1)b_t]X_t. \quad (70)$$

Numerical values of the a_t and b_t expansion coefficients have already been obtained (Bessis *et al* 1982). Hence, closed-form expressions for the bound-state energies $E_{jm}^{(1)}$ can be obtained in terms of the analytical expressions of the class II ($\varepsilon=-1$) matrix elements $X_0(s)$ (see equation (40)) and $X_t=\langle j\,m|[\tan(ax/2)]^t|j\,m\rangle$ where $d=-[(A+\frac{1}{4})^{1/2}+l+\frac{1}{2}]/2$; $m=[(A+\frac{1}{4})^{1/2}-l-\frac{3}{2}]$ and $j=m-n$. Of course, the accuracy of the result depends on the truncation (in t) of expression (70) and also on the particular choice of effective parameters in the expression for the unperturbed Hamiltonian (see Bessis *et al* 1982).

Among other possible interesting applications, let us mention that the algebraic recursive procedure can also be of some practical interest for an analytical perturbative treatment of the Schrödinger equation with the Hulthen potential $V_H(x)$

$$\{d^2/dx^2-l(l+1)/x^2+Z\beta\exp(-\beta x)/[1-\exp(\beta x)]+2E\}\Psi(x)=0 \quad (71)$$

with the associated boundary conditions $\Psi(0)=\Psi(\infty)=0$.

Indeed, noting that the Hulthen potential $V_H(x)$ can be rewritten as

$$V_H(x)=-Z\beta[\coth(\beta x/2)-1]/2$$

and that the rotational term x^{-2} behaves as $[(2/\beta)\sinh(\beta x/2)]^{-2}$, a suitable unperturbed eigenequation is

$$[\mathrm{d}^2/\mathrm{d}x^2-\beta^2 l(l+1)/4\sinh^2(\beta x/2)+2Z\beta\coth(\beta x/2)-Z\beta+2E^{(0)}]\Psi^{(0)}=0. \qquad (72)$$

One easily recognises a type-E factorisable equation (43) with $A=\mathrm{i}\beta/2$.

Let us add that, in the same way, the Schrödinger equation with the exponentially screened static Coulombic potential $V_{sc}(x)_= = -Z\exp(-\alpha x)/x$ can also be regarded as an unperturbed type-E factorisable eigenequation with additional perturbations after noting that the Hulthen potential $V_H(x)$ may constitute a rather good unperturbed approximation to the screened potential $V_{sc}(x)$.

The above examples have been given to illustrate how the algebraic recursive procedure would be useful for an analytic perturbative treatment of many model eigenequations, within the classical Rayleigh–Schrödinger scheme, and the computation of associated expectation values. Of course, although it is well adapted for computer programs which perform algebraic manipulations, such as REDUCE (Hearn 1976) or MACSYMA (1977), for an accurate treatment of the above eigenequations, up to a high order of the perturbation, the shifted $1/N$ expansion method (see, for instance, Dutt *et al* 1986 and references therein) and/or the perturbed ladder operator method (Bessis *et al* 1983 and references therein) remain more attractive.

6. Conclusion

Finally, it has been shown how the combined use of different ladder relations satisfied by the $\Psi_j^m(x)$ eigenfunctions and by naturally adapted sets of $Q_t(x)$ functions provides recurrence formulae for calculating matrix elements between solutions of factorisable equations. As a consequence, closed-form expressions for the diagonal ($j'=j$, $m'=m$) matrix elements can be obtained from the knowledge of very few classical integrals which, in most cases, can be found in tables or even without having to perform any integration. It is no longer necessary to consider separately the determination of class I or class II matrix elements according to the boundary conditions of the problem: one obtains unified expressions containing the binary class parameter ε. It has been shown how the range of applicability of the procedure, i.e. the field of suitable $Q_t(x)$, can be enlarged by using the connection between factorisation types and, also, how the recursive procedure can be extended to the determination of off-diagonal matrix elements (in terms of the diagonal ones) by a repeated use of the ladder operators to the bra (or ket) $\Psi_j^m(x)$ eigenfunctions.

Recurrence formulae (14) or (16) are valid for all factorisation types. They can be used, for instance, for calculating matrix elements of $Q_t(x)=\exp[-(p+t)x+qe^x]$ between type-B eigenfunctions which are related to the confluent hypergeometric functions and, particularly, are of some interest in diatomic vibration studies within the perturbed Morse potential model (see, for instance, Badawi *et al* 1973 and Huffaker and Dwivedi 1975). In that case, the choice of suitable $Q_t(x)$ functions can be still enlarged by using the interconnection between type-B and type-F factorisations. Since most of expansion basis functions of current use in quantum physics are connected by simple relations either with the Gaussian or the confluent hypergeometric functions, the algebraic recursive procedure may constitute a useful and efficient tool for computing expectation values and, also, for an analytic perturbative treatment of many model eigenequations within the classical Rayleigh–Schrödinger scheme.

In the present paper, we have focused our attention on the determination of matrix elements between the transformed Jacobi eigenfunction, and closed-form expressions have been obtained for matrix elements of $Q_t(x) = [\tan(ax/2)]^t$ and $Q_t(x) = (\cos ax)^t$. Of course, alternative expressions for matrix elements between the transformed Jacobi eigenfunctions are obtainable (Bessis *et al* 1982) by using the orthonormality property of the eigenfunctions after expanding the Jacobi polynomials $P_v^{(\alpha,\beta)}(y)$ on the finite basis of the $P_k^{(a,b)}(y)$

$$P_v^{(\alpha,\beta)}(y) = \sum_{k=0}^{v} C_k^{(v)} P_k^{(a,b)}(y)$$

where $y = \cos(ax)$ and (see Miller 1968)

$$\begin{aligned} C_k^{(v)} = [&\Gamma(\alpha+\beta+v+k+1)\Gamma(a+b+k+1)\Gamma(\alpha+v+1)/(v-k)!\Gamma(\alpha+\beta+v+1) \\ &\times \Gamma(a+b+2k+1)\Gamma(\alpha+k+1)] \\ &\times {}_3F_2(k-v, \alpha+\beta+v+k+1, a+1; \alpha+k+1, a+b+2k+2; 1). \end{aligned}$$

The use of this expansion in a term-wise integration leads to closed-form expressions involving hardly reducible summations (with upper bound $v = \varepsilon(j-m)$) which may conceal a simpler analytical dependence in the quantum numbers j and m (see equations (33)-(36) or (55) and (56)) and, from a computational point of view, the use of the algebraic recursive procedure is, by far, more advantageous.

Appendix 1. Calculation of particular type-A matrix elements

A1.1. Class I $X_2 = \langle j\, m|\, [\tan(ax/2)]^2 |j\, m\rangle$ matrix elements

Setting $\cos ax = y$ and noting that $[\tan(ax/2)]^2 = (1-y)/(1+y) = -1 + 2/(1+y)$, one can write

$$X_2 = -1 + 2\int_{-1}^{1} (1-y)^{\alpha}(1+y)^{\beta-1}|P_v^{(\alpha,\beta)}(y)|^2\,\mathrm{d}y \times\left(\int_{-1}^{1} (1-y)^{\alpha}(1+y)^{\beta}|P_v^{(\alpha,\beta)}(y)|^2\,\mathrm{d}y\right)^{-1}. \tag{A1.1}$$

Closed-form expressions for both integrals involved in (A1.1) can be obtained from tables in Gradshteyn and Ryzhik (1980)

$$\int_{-1}^{1} (1-y)^{\alpha}(1+y)^{\beta}|P_v^{(\alpha,\beta)}(y)|^2\,\mathrm{d}y = (2^{\alpha+\beta+1}\Gamma(\alpha+v+1)\Gamma(\beta+v+1))/v!(\alpha+\beta+2v+1)\Gamma(\alpha+\beta+v+1) \tag{A1.2}$$

and

$$\int_{-1}^{1} (1-y)^{\alpha}(1+y)^{\beta-1}|P_v^{(\alpha,\beta)}(y)|^2\,\mathrm{d}y = (2^{\alpha+\beta}\Gamma(\alpha+v+1)\Gamma(\beta+v+1))/v!\beta\Gamma(\alpha+\beta+v+1). \tag{A1.3}$$

Hence, one obtains

$$X_2 = -1 + (\alpha+\beta+2v+1)/\beta. \tag{A1.4}$$

Using the expressions (22) and (19) for α, β, and v, one gets the class I expression (43) of X_2.

A1.2. Class II $X_2 = \langle j\, m|[\tanh(|a|x/2)]^2|j\, m\rangle$ matrix elements

Setting $z = \cosh|a|x$ and noting that $[\tanh(|a|x/2)]^2 = 1 - 2/(z+1)$, one can write

$$X_2 = 1 - 2\int_1^\infty (z-1)^\alpha (z+1)^{\beta-1}|P_v^{(\alpha,\beta)}(z)|^2\, dz$$
$$\times\left(\int_1^\infty (z-1)^\alpha (z+1)^\beta |P_v^{(\alpha,\beta)}(z)|^2\, dz\right)^{-1}. \tag{A1.5}$$

The expression of the normalisation integral in (A1.5) has already been obtained in a previous paper (Bessis *et al* 1982) and can be rewritten as

$$\int_1^\infty (z-1)^\alpha (z+1)^\beta |P_v^{(\alpha,\beta)}(z)|^2\, dz$$
$$= [2^{\alpha+\beta}\Gamma(\alpha+v+1)\Gamma(\beta+v+1)]\sin\beta\pi/[v!\beta(\alpha+\beta+2v+1)$$
$$\times\Gamma(\alpha+\beta+v+1)\sin(\alpha+\beta)\pi]. \tag{A1.6}$$

Let us remark that, for both classes, the expressions of the other integral in (A1.5) can be expressed in terms of a normalisation integral involving the $P_v^{(\alpha,\beta-1)}(z)$ Jacobi polynomial. Indeed, one can use the following relation (see, for instance, Miller 1968):

$$P_v^{(\alpha,\beta)}(z) = \sum_{k=0}^{v} w_k^{(v)} P_v^{(\alpha,\beta-1)}(z) \tag{A1.7}$$

where

$$w_k^{(v)} = (-1)^{v-k}(\alpha+\beta+2k)\Gamma(\alpha+\beta+k)\Gamma(\alpha+v+1)/\Gamma(\alpha+\beta+v+1)\Gamma(\alpha+k+1)$$

and, owing to the orthogonality property of the Jacobi eigenfunctions, one gets, for class I and class II respectively,

$$\int_{-1}^{+1} (1-y)^\alpha (1+y)^{\beta-1}|P_v^{(\alpha,\beta)}(y)|^2\, dy$$
$$= \sum_{k=0}^{v} (w_k^{(v)})^2 \int_{-1}^{1} (1-y)^\alpha (1+y)^{\beta-1}|P_k^{(\alpha,\beta-1)}(y)|^2\, dy \tag{A1.8}$$

$$\int_1^\infty (z-1)^\alpha (z+1)^{\beta-1}|P_v^{(\alpha,\beta)}(z)|^2\, dz$$
$$= \sum_{k=0}^{v} (w_k^{(v)})^2 \int_1^\infty (z-1)^\alpha (z+1)^{\beta-1}|P_k^{(\alpha,\beta-1)}(z)|^2\, dz. \tag{A1.9}$$

Hence, using comparatively the expressions (A1.2) and (A1.6), one finally obtains

$$\int_1^\infty (z-1)^\alpha (z+1)^{\beta-1}|P_v^{(\alpha,\beta)}(z)|^2\, dz\left(\int_1^\infty (z-1)^\alpha (z+1)^\beta |P_v^{(\alpha,\beta)}(z)|^2\, dz\right)^{-1}$$
$$= (\alpha+\beta+2v+1)/(2\beta) \tag{A1.10}$$

and, consequently, for class II matrix elements (see equation (A1.5))

$$X_2 = -(\alpha+2v+1)/\beta \tag{A1.11}$$

or, after using the class II ($\varepsilon = -1$) expressions (22) for α, β and v, one gets the class II expression (32) for X_2.

A1.3. Class I and class II $\langle j\,m|[\cos(ax/2)]^{-2s}|j\,m\rangle$ matrix elements

For class I problems, closed-form expressions for $X_0(s)$ and of $X_2(s)$ can be derived from tables in Erdélyi (1954). Indeed, after setting $y = \cos ax$, one can write

$$[\cos(ax/2)]^{-2s}[\tan(ax/2)]^2 = -[2/(1+y)]^s + [2/(1+y)]^{s+1}.$$

Thus, $X_2(s) = -X_0(s) + X_0(s+1)$ and it is sufficient to evaluate $X_0(s)$, i.e.

$$X_0(s) = 2^s \int_{-1}^{1} (1-y)^\alpha (1+y)^{\beta-s} |P_v^{(\alpha,\beta)}(y)|^2 \, \mathrm{d}y \times \left(\int_{-1}^{1} (1-y)^\alpha (1+y)^\beta |P_v^{(\alpha,\beta)}(y)|^2 \, \mathrm{d}y \right)^{-1}. \quad \text{(A1.12)}$$

The computation of the above (class I) integral involving s is somewhat more intricate than the computation of integral (A1.3); nevertheless it can be still obtained from tables in Erdélyi (1954)

$$X_0(s) = [(\alpha+\beta+2v+1)\Gamma(s+v)\Gamma(\alpha-s+1)\Gamma(\alpha+\beta+v+1)/v!$$
$$\Gamma(\alpha+1)\Gamma(s)\Gamma(\alpha+\beta-s+v+2)]$$
$$\times {}_4F_3(-v, \alpha+\beta+v+1, \alpha-s+1, -s+1;$$
$$\alpha+1, \alpha+\beta-s+v+2, -s-v+1; 1). \quad \text{(A1.13)}$$

For class II ($\varepsilon = -1$) problems, the same considerations as for the $X_t(s=0)$ matrix elements lead to the closed-form expression for any $X_t(s)$ matrix element from the knowledge of its class I counterpart (substitute $(j+1)$ with j and change the sign overall); after introducing the class parameter ε, one gets the expression (40) for $X_0(s)$, which is valid for both classes.

Appendix 2. Determination of the normalisation conversion factor

The normalsiation conversion factor $C = C(j, m)$ is defined, in terms of a diagonal type-E matrix element, by the following relation (see equations (6) and (41)):

$$ba^{-1}C^2\langle J\,M|(a\cosh b\chi)^{-2}|J\,M\rangle = 1 \quad \text{(A2.1)}$$

or, in the standard type-E notation

$$-(ab)^{-1}C^2\langle J\,M|A^2/\sin^2 A(\chi+\chi_0)|J\,M\rangle = 1. \quad \text{(A2.2)}$$

For class I and $a = 1$, this matrix element have been obtained in closed form in a previous paper (Bessis *et al* 1984). It is worthwhile to present here a unified and consistent technique for deriving a unified expression of this matrix element from ladder operator considerations.

Let us consider the following alternative expressions of $A\cot A(\chi+\chi_0)$ as proper combinations of the type-E ladder operators $\mathfrak{H}_M^- = AM\cot A(\chi+\chi_0) + Q/M - \mathrm{d}/\mathrm{d}\chi$, i.e.

$$A\cot A(\chi+\chi_0) = Q/M^2 + (\mathfrak{H}_M^+ + \mathfrak{H}_M^-)/2M$$
$$= Q/(M-1)^2 + (\mathfrak{H}_{M-1}^+ + \mathfrak{H}_{M-1}^-)/2(M-1). \quad \text{(A2.3)}$$

Using the ladder equations (45) together with the mutual adjointness property of $\mathfrak{H}_M^+$ and $\mathfrak{H}_M^-$ operators, one can write alternative expressions for a same matrix element involving any differentiable function $G(\chi)$

$$\begin{aligned}
\langle J\, M-1|G(\chi)A \cot A(\chi+\chi_0)|J\, M-1\rangle
&= (Q/M^2)\langle J\, M-1|G|J\, M-1\rangle - (1/2M)\langle J\, M-1|\, \mathrm{d}G/\mathrm{d}\chi|J\, M-1\rangle \\
&\quad + (\Lambda_J(M)/M)\langle J\, M-1|G|J\, M\rangle \\
&= (Q/(M-1)^2)\langle J\, M-1|G|J\, M-1\rangle \\
&\quad + [1/2(M-1)]\langle J\, M-1|\mathrm{d}G/\mathrm{d}\chi|J\, M-1\rangle \\
&\quad + [\Lambda_J(M-1)/(M-1)]\langle J\, M-2|G|J\, M-1\rangle. \qquad \text{(A2.4)}
\end{aligned}$$

First, setting $G(\chi)=1$ in (A2.4), one gets

$$\begin{aligned}
\langle J\, M-1|A \cot A(\chi+\chi_0)|J\, M-1\rangle
&= (Q/M^2) + [\Lambda_J(M)/M]\langle J\, M-1|J\, M\rangle \\
&= (Q/(M-1)^2) + (\Lambda_J(M-1)/(M-1))\langle J\, M-2|J\, M-1\rangle. \qquad \text{(A2.5)}
\end{aligned}$$

Therefore, this matrix element must be independent of M and, since $\Lambda_J(J+\bar{\varepsilon}/2+\frac{1}{2})=0$, after setting $M=J+\bar{\varepsilon}/2+\frac{1}{2}$ in (A2.5), one gets

$$\langle J\, M|A \cot A(\chi+\chi_0)|J\, M\rangle = Q/(J+\bar{\varepsilon}/2+\tfrac{1}{2})^2 \qquad \text{(A2.6)}$$

where $\bar{\varepsilon}=-\varepsilon$ is the type-E class parameter.

Setting in (A2.4)

$$G(\chi)=A \cot A(\chi+\chi_0), \quad G(\chi)A \cot A(\chi+\chi_0) = -A^2 + A^2/\sin^2 A(\chi+\chi_0)$$

and using (A2.6), one gets, after some rearrangements

$$\begin{aligned}
(M-\tfrac{1}{2})\langle J\, M-1|A^2/\sin^2 A(\chi+\chi_0)|J\, M-1\rangle
&= A^2M + [Q^2/M(J+\bar{\varepsilon}/2+\tfrac{1}{2})^2] + \Lambda_J(M)\langle J\, M-1|A \cot A(\chi+\chi_0)|J\, M\rangle \\
&= A^2(M-1) + [Q^2/(M-1)(J+\bar{\varepsilon}/2+\tfrac{1}{2})^2] \\
&\quad + \Lambda_J(M-1)\langle J\, M-2|A \cot A(\chi+\chi_0)|J\, M-1\rangle. \qquad \text{(A2.7)}
\end{aligned}$$

Using the same arguments as above, one gets

$$(M+\tfrac{1}{2})\langle J\, M|A^2/\sin^2 A(\chi+\chi_0)|J\, M\rangle = A^2(J+\bar{\varepsilon}/2+\tfrac{1}{2}) + Q^2/(J+\bar{\varepsilon}/2+\tfrac{1}{2})^3 \qquad \text{(A2.8)}$$

and, in terms of the original type-A quantum numbers j, m and class parameter $\varepsilon=-\bar{\varepsilon}$, one obtains

$$C^2(j,m) = ab^{-1}(j+\varepsilon+\tfrac{1}{2})(m+\tfrac{1}{2})/[(m+\tfrac{1}{2})^2-d^2]. \qquad \text{(A2.9)}$$

Appendix 3. Some particular type-A eigenfunctions

A3.1. Associated spherical harmonics

$$Y_L^M(\theta,\phi) = (2\pi)^{-1/2}\exp(\mathrm{i}M\varphi)(\sin\theta)^{-1/2}\Psi_{LM}(\theta).$$

$\Psi_L^M(\theta)$ is a class I ($\varepsilon=1$) solution of eigenequation (17) with $x=\theta$, $0\leqslant\theta\leqslant\pi$; $a=1$; $d=0$; $j=L-\frac{1}{2}$; $m=M-\frac{1}{2}$ and $L-M=j-m=$ positive integer or zero.

A3.2. Symmetric top functions

$$D^{(L)}_{M,K}(\alpha, \beta, \gamma) = \exp(\mathrm{i}M\alpha) d^{(L)}_{MK}(\beta) \exp(\mathrm{i}K\gamma)$$

where α, β, γ are the three Euler angles: $0 \leqslant \alpha \leqslant 2\pi$; $0 \leqslant \beta \leqslant \pi$; $0 \leqslant \gamma \leqslant 2\pi$,

$$d^{(L)}_{MK}(\beta) = [2/(2l+1)]^{1/2}(\sin\beta)^{-1/2}\Psi_{LM}(\beta)$$

with $\Psi_{LM}(\beta)$ being a class I ($\varepsilon = 1$) solution of eigenequation (17) with $x = \beta$; $a = 1$; $j = L - \frac{1}{2}$. Since both differences $L - M$ and $L - K$ are positive integers or zero, $\Psi_{LM}(\beta)$ is a type-A eigenfunction either when setting $M = m + \frac{1}{2}$ and $K = d$, or when setting $M = d$ and $K = m + \frac{1}{2}$.

A3.3. Gauss hypergeometric functions

The differential equation satisfied by the Gauss hypergometric function ${}_2F_1(\alpha, \beta; \gamma; z)$ is (Gradshteyn and Ryzhik 1980)

$$\{z(1-z)\mathrm{d}^2/\mathrm{d}z^2 + [\gamma - (\alpha+\beta+1)z]\,\mathrm{d}/\mathrm{d}z - \alpha\beta\}F(z) = 0.$$

Setting $z = \sin^2 x$ and $F = (\sin x)^{-\gamma+1/2}(\cos x)^{-\alpha-\beta+\gamma-1/2}\Psi(x)$, one obtains

$$[\mathrm{d}^2/\mathrm{d}x^2 - 4(m^2 + d^2 - \tfrac{1}{4} + 2md\cos 2x)/\sin^2 2x + (\alpha-\beta)^2]\Psi(x) = 0$$

where $m = (\alpha + \beta - 1)/2$ and $d = (2\gamma - \alpha - \beta - 1)/2$.

$\Psi(x)$ is a class I ($\varepsilon = 1$) solution of eigenequation (17) with $a = 2$, $\lambda_j = (\alpha - \beta)^2$. On the other hand, the quantisation condition requires $j - m = v$ = positive integer and $\lambda_j = L(j+1) = L(m+v+1) = 4(v + (\alpha+\beta)/2)^2$. As a consequence, either $\alpha = -v$ or $\beta = -v$, i.e. one finds again the well known condition for finite hypergeometric series.

References

Badawi M, Bessis N and Bessis G 1973 *Can. J. Phys.* **51** 2075
Bessis N and Bessis G 1987 *J. Phys. A: Math. Gen.* **20** 5745
Bessis N, Bessis G and Hadinger G 1983 *J. Phys. A: Math. Gen.* **16** 497
Bessis N, Bessis G and Joulakian B 1982 *J. Phys. A: Math. Gen.* **15** 3679
Bessis N, Bessis G and Shamseddine R 1984 *Phys. Rev.* A **29** 2375
Buck B 1977 *Nucl. Phys.* A **275** 246
Dutt R, Mukherji U and Varshni Y P 1986 *J. Phys. B: At. Mol. Phys.* **19** 3411
Erdélyi A, Magnus W, Oberhettinger F and Tricomi F 1954 *Tables of Integral Transforms* vol 2 (New York: McGraw-Hill)
Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic)
Hadinger G, Bessis N and Bessis G 1974 *J. Math. Phys.* **15** 716
Hearn A C 1971 *Commun. ACM* **14** 511
Huffaker J N and Dwivedi P H 1975 *J. Math. Phys.* **16** 862
Infeld L and Hull T E 1951 *Rev. Mod. Phys.* **23** 21
Lai C S 1983 *J. Phys. A: Math. Gen.* **16** L181
1977 MACSYMA *Reference Manual* (Cambridge, MA: Laboratory of Computer Science, Massachusetts Institute of Technology)
Miller W Jr 1968 *J. Math. Phys.* **9** 1163
Schrödinger E 1940 *Proc. R. Irish Acad.* A **46** 183
—— 1941 *Proc. R. Irish Acad.* A **47** 53
Stephenson G 1977 *J. Phys. A: Math. Gen.* **10** 1229