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Some properties of the five-dimensional surface harmonics

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Abstract

Ladder operators and a triangular relation are used to derive the five-dimensional surface harmonics with definite angular momentum, as used in studies of the dynamics of a quadrupole shape in the nuclear collective model. A new basis is used which leads to solutions in terms of associated Legendre functions. The role of the Octahedral symmetry group and the limit of large quantum numbers are discussed.

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1. Introduction

In three dimensions, the surface harmonics $Y_{lm}(\theta, \phi)$ provide a useful complete set of functions of the polar angles θ, ϕ while the functions $\psi = r^l Y_{lm}(\theta, \phi)$ and $r^{-(l+1)} Y_{lm}(\theta, \phi)$ are solutions of the Laplace equation $\nabla^2\psi = 0$. The operator ∇^2 separates into a radial part $r^{-2}\partial/\partial r(r^2\partial/\partial r)$ and an angular part $-\Lambda/r^2$ so that Y_{lm} is an eigenfunction of Λ with eigenvalue $l(l+1)$. Group theoretically, the Y_{lm} provide a basis for the irreducible representation D_l of the rotation group $O(3)$ and Λ is the Casimir operator.

A similar situation occurs in five dimensions and is of interest because many properties of atomic nuclei can be understood as the motions, such as rotation and vibration, of a quadrupole shape, which requires five variables to define it. A convenient choice of variables is obtained by introducing the principal axes of the shape which require three Euler angles, denoted Ω, to define their orientation relative to the laboratory frame, leaving two variables β and γ to define the intrinsic shape. In detail, β and γ are conventionally defined by giving the radial distance from the centre of the shape to its boundary as

$$R(\theta, \varphi) = R_0\left[1 + \beta\cos\gamma Y_{20}(\theta, \phi) + \sqrt{\tfrac{1}{2}}\beta\sin\gamma\{Y_{22}(\theta, \varphi) + Y_{2-2}(\theta, \phi)\}\right] \tag{1}$$

where θ and ϕ refer to the principal axes. Thus β, running from zero to infinity, describes the overall deformation from spherical at $\beta = 0$, and is analogous to the radius r in three dimensions while γ is the single shape variable and runs from zero to $\pi/3$. The use of larger values of γ only reproduces the same range of shapes but with a different labelling of axes.

In five dimensions therefore we again have a single radial variable β with four angles, γ and the three Euler angles Ω. The five-dimensional Laplacian again separates into a radial part $\beta^{-4}\partial/\partial\beta(\beta^4\partial/\partial\beta)$ and an angular part $-\Lambda/\beta^2$ and it follows that a set of solutions of the Laplace equation may be written as

$$\beta^{\lambda}Y_{\lambda\alpha}(\gamma,\Omega) \qquad \text{and} \qquad \beta^{-(\lambda+3)}Y_{\lambda\alpha}(\gamma,\Omega).$$

The $Y_{\lambda\alpha}$ are eigenfunctions of Λ with eigenvalues $\lambda(\lambda+3)$, and for each λ they form the basis of an irreducible representation $(\lambda, 0)$ of the group $O(5)$ where Λ is the Casimir operator. (We have used the same symbols Λ and Y in both the three- and five-dimensional cases, to emphasize the analogy, but in the rest of the paper these symbols always refer to five dimensions.) In three dimensions the familiar label m on the spherical harmonic is sufficient to label all solutions with a given l and it denotes the representation of the subgroup $O(2)$ of $O(3)$. In five dimensions there is a greater variety of subgroups of $O(5)$ from which to choose a labelling system for the basis of the $O(5)$ representation. We have denoted these labels symbolically by α. It is important to choose the physical $O(3)$, relating to the quadrupole shape described above, as a subgroup since this provides angular-momentum labels IM for the motion of the shape. In general I and M are not sufficient to label all basis vectors of $(\lambda, 0)$ so we retain a label α in addition to IM.

It is well known that, in three dimensions, the surface harmonic Y_{lm} is given explicitly as an associated Legendre function $P_l{}^m(\cos\theta)$, together with a factor $\exp(im\phi)$ and some conventional phase and normalization. In five dimensions the explicit form of the $Y_{\lambda\alpha IM}$ was first given only for particular small I and λ by Bès [1] in 1959 and for $I = 2$ with any λ by Budnik *et al* [2] but general formulae were given in two papers by Chacón *et al* [3] in about 1977. Here we revisit the problem of constructing these solutions. Section 2 discusses symmetries and describes the array of solutions as well as introducing several algebraic devices, which include ladder operators and a triangular relation. Section 3 re-derives the earlier results [3] more directly, using a recurrence relation. A completely new basis is used to derive the solutions in section 4 with the coefficients being given in terms of a few Legendre functions. Section 5 considers the limit of large λ. Some $B(E2)$ values are calculated in section 6 and compared with the results at large λ The transition from even I to odd I is briefly described in section 7. Appendices A and B contain proofs of some results quoted in the paper while C and D give the complete set of solutions and norms for $I \leqslant 8$. The use of irreducible representations of the Octahedral group rather than the rotation matrices D^I_{MK} is discussed in section 4.4 and in appendix E.

2. General properties of the solutions

2.1. Symmetries and the basis

To achieve states with definite angular momentum I and with projection M on the laboratory z-axis we must use the rotation matrices $D^I_{MK}(\Omega)$ of the Euler angles Ω but their use to define the intrinsic frame implies that certain symmetries must be satisfied. The labelling xyz of the axes is non-physical and hence [4] any wavefunctions must be invariant under the Octahedral group which permutes the labels. These group operations affect both γ and the Ω. Although γ is invariant under the subgroup D_2 of π-rotations, we can only ensure D_2-invariance for the Ω-dependence if the D-functions are used in the combinations

$$\Phi_{IMK} = \left(D^I_{MK} + (-1)^I D^I_{M-K}\right)\Big/\sqrt{2(1+\delta_{K,0})} \qquad (2)$$

with even $K \geqslant 0$. The general solution may then be written as

$$Y_{\lambda\alpha IM} = \sum_K f_{IK}(\gamma)\Phi_{IMK} \tag{3}$$

which is the form originally used by Bès. However, we know that the solutions must have overall invariance with respect to the Octahedral group and the calculation of the coefficients f is simplified by constructing, in place of the Φ_{IMK}, a basis which is invariant under the Octahedral group. The coefficients are then functions only of the invariant $\cos 3\gamma$. This technique has been used in the more recent papers [3].

The basis is constructed from the building blocks Φ_{220} and Φ_{222}. Clearly, any product of n such factors has total $M = 2n$ and, from the usual angular-momentum coupling rules, the total angular momentum I cannot exceed $2n$. Hence $I = 2n$. In other words, any product of $I/2$ automatically has angular momentum I. The fact that it has a specific $M = I$ is unimportant since, if required, the M-dependence in (3) is contained in the known D-functions. This argument clearly applies only to even I but the extension to odd I is straightforward and will be discussed later, in section 7.

The functions Φ_{220} and Φ_{222} can be shown to belong to the representation E of the Octahedral group. (The irreducible representations of the Octahedral group are labelled A_1 (invariant), A_2 (one-dimensional), E (two-dimensional) and T_1, T_2 (three-dimensional).) Thus, to form an Octahedral invariant for $I = 2$, this pair must be combined with functions of γ as coefficients, which also transform according to E, so that the sum becomes invariant. The simplest invariant combinations, and those used in previous work, are

$$\phi_+ = \cos\gamma\,\Phi_{220} + \sin\gamma\,\Phi_{222} \qquad \text{and} \qquad \phi_0 = \cos 2\gamma\,\Phi_{220} - \sin 2\gamma\,\Phi_{222}. \tag{4}$$

They are orthogonal when the proper integration over γ is carried out. In later sections of this paper we explore the use of an alternative to ϕ_0.

2.2. *The ladder operators*

For the simplest case $I = 0$, there is no dependence on Ω and we only need the appropriate function of $x = \cos 3\gamma$. The Casimir operator Λ in this case reduces to $-9\partial/\partial x(1 - x^2)\partial/\partial x$ which is a multiple of the Legendre operator. The eigenfunctions are therefore the Legendre polynomials $f = P_l(x)$ with eigenvalues $9l(l+1) = 3l(3l+3)$ corresponding to $\lambda = 3l$ in the previous notation with $l = 0, 1, 2$, etc. We now show how to construct ladder operators which generate any $Y_{\lambda\alpha}$ starting from these $I = 0$ solutions. (To simplify the notation we henceforth omit the label $M = I$.)

By definition, the harmonics $\psi = \beta^\lambda Y_{\lambda\alpha}$ and $\psi = \beta^{-(\lambda+3)} Y_{\lambda\alpha}$ satisfy the five-dimensional Laplace equation $\nabla^2\,\psi = 0$. From the elementary Cartesian form for ∇^2, it is immediate that the derivative operator $\partial/\partial\alpha_\nu$ commutes with ∇^2 where a_ν is any of the Cartesian co-ordinates in five dimensions defined in equation (7) below. Hence it follows, from the usual symmetry argument that, in particular, $\partial\psi/\partial a_{-2}$ is also a harmonic.

But $\partial/\partial a_{-2}$ has dimension β^{-1} in the radial variable so that we must have

$$\frac{\partial}{\partial a_{-2}}\beta^\lambda Y_{\lambda\alpha} = \beta^{\lambda-1} Y_{\lambda-1\alpha'} \qquad \text{and} \qquad \frac{\partial}{\partial a_{-2}}\beta^{-(\lambda+3)} Y_{\lambda\alpha} = \beta^{-(\lambda+4)} Y_{\lambda+1\alpha'}.$$

The powers of β may quickly be eliminated to give the dimensionless ladder operators $Q_\pm(\lambda)$ defined by

$$Y_{\lambda-1\alpha'} = Q_-(\lambda)Y_{\lambda\alpha} = \{\lambda\partial\beta/\partial a_{-2} + \beta\partial/\partial a_{-2}\}Y_{\lambda\alpha} \tag{5}$$

$$Y_{\lambda+1\alpha'} = Q_+(\lambda)Y_{\lambda\alpha} = \{-(\lambda+3)\partial\beta/\partial a_{-2} + \beta\partial/\partial a_{-2}\}Y_{\lambda\alpha}. \tag{6}$$

These equations define the normalizations and labels α' of the new harmonics on the left in terms of the original $Y_{\lambda\alpha}$ on the right. Importantly, however, if we choose the original harmonic to have angular momentum I with maximum projection $M = I$, it follows that the harmonics on the left also have a definite angular momentum $I + 2$ with maximum projection $I + 2$. Using an earlier argument, this is an immediate consequence of the property that the operator $\partial/\partial a_{-2}$ increases the angular-momentum projection M in the laboratory frame by two units. Hence, equations (5) and (6) show that the operators on the right not only change λ by one unit but also remain within the set of states with maximum $M = I$, increasing both M and I by two units. It is therefore possible to start from the $I = 0$ solution discussed above, for a particular l, and to generate a family of harmonics with increasing even I which all carry the same additional label l. Thus l can be used for both the additional labels α and α'.

To make practical use of this idea for constructing the $Y_{\lambda Il}$ we must find the effect of the Cartesian derivative $\partial/\partial a_{-2}$ when acting on the polar variables β, γ and the building blocks (4). To this end, we now collect together some elementary results.

The five Cartesian co-ordinates, with laboratory frame components μ, are conventionally written as

$$a_\mu = \beta(\cos\gamma\,\Phi_{2\mu0} + \sin\gamma\,\Phi_{2\mu2}) \tag{7}$$

so that, in particular, $a_2 = \beta\phi_+$. Similarly, the second of the functions (4) is given by the tensor product

$$(a\times a)^{(2)}_2 = -\sqrt{\tfrac{2}{7}}\beta^2\phi_0. \tag{8}$$

The quadratic and cubic invariants are given by

$$\beta^2 = \sum_\upsilon (-1)^\upsilon a_\upsilon a_{-\upsilon} \tag{9}$$

$$\beta^3\cos 3\gamma = -\sqrt{\tfrac{35}{2}}(a\times a\times a)^0_0 \tag{10}$$

from which we deduce the derivatives

$$\partial\beta/\partial a_{-2} = \phi_+ \tag{11}$$

$$\beta\partial(\cos 3\gamma)/\partial a_{-2} = 3(\phi_0 - \cos 3\gamma\,\phi_+) \tag{12}$$

$$\beta\partial\phi_+/\partial a_{-2} = -(\phi_+)^2 \tag{13}$$

$$\beta\partial\phi_0/\partial a_{-2} = -2\phi_+\phi_0. \tag{14}$$

2.3. The array of solutions

It is convenient to picture the solutions for all even I as an array in the two dimensions I and λ as shown in figure 1. Starting from a solution with $I = 0$ and $\lambda = 3l$, at the bottom of the figure, we may construct the family of solutions labelled l by first acting a number n_- times with the lowering operator (5) and then a number n_+ times with the raising operator (6). To reach a particular point λ, I in the figure these numbers are given by $n_+ + n_- = I/2$, and $n_+ - n_- = \lambda - 3l$. This path is obviously not unique but other paths lead to the same solution. To show this we use the ladder operators introduced in (5) and (6) which, from (11) and (12), satisfy the relation

$$Q_+(\lambda-1)Q_-(\lambda) = Q_-(\lambda+1)Q_+(\lambda).$$

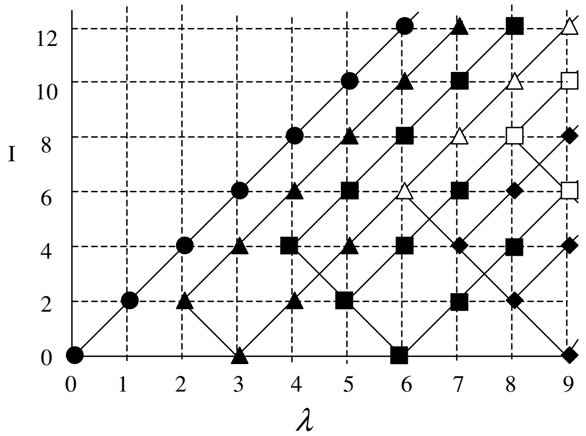

Figure 1. The array of solutions for even I. Non-degenerate solutions with $l = 0$, 1, 2 and 3 are denoted by black circles, triangles, squares and diamonds respectively. The white shapes denote cases that are doubly degenerate due to the overlap of a band of solutions with the indicated l and another having $l + 2$. Thus, for example, there are two solutions at $I = \lambda = 6$ with $l = 1$ and 3. The band of solutions with maximum λ for a given l, namely $I = 2(\lambda - 3l)$, is the 'top-band'.

This shows the equivalence of the paths around the left- or right-hand sides of a small square in figure 1, from which the more general conclusion follows. However, n_- must not exceed l since otherwise a solution belonging to a family with smaller l is produced, see appendix A. There is no upper limit to n_+. Some points on the grid may be reached in this way starting from more than one value of l. In such cases, there is more than one independent solution with the same I and λ and different l so that l serves as the multiplicity label to distinguish them. Most of the points in the region shown in figure 1 have a unique l-value but those with a multiplicity of two are shown as white shapes.

Figure 1 demonstrates that the complete set of solutions has a band structure labelled by n_-. With the $O(5)$ Casimir operator in the Hamiltonian, the energy spectrum behaves like $\lambda(\lambda + 3)$ so that the energy increases along the horizontal axis of the figure. The $n_- = 0$ bands have $I = 0, 2, 4, \ldots$, the $n_- = 1$ bands have $I = 2, 4, 6, \ldots$ etc, which is the same set of even values as in a rotational band with $K = 2n_-$. For each value of n_-, the label l runs from n_- to ∞.

Some simple rules for the allowed values of l and I follow from the definitions of n_+ and n_- and their limits $n_+ \geqslant 0$, $0 \leqslant n_- \leqslant l$, discussed above. For example, given λ, the integer l runs from zero and must not exceed $\lambda/2$ while, for each λ and l, the range of angular momentum is given by

$$2|\lambda - 3l| \leqslant I \leqslant 2(\lambda - l)$$

where I moves by steps of 4. For given λ and I, these inequalities imply that the multiplicity label l is confined to the range

$$(\lambda - I/2)/3 \leqslant l \leqslant \min\{(\lambda - I/2), (\lambda + I/2)/3\}.$$

However, we must add to this inequality the constraint that l must be even (odd) accordingly as $(\lambda - I/2)$ is even (odd) which also follows from the definition of n_+ and n_-. (Recall that this discussion is restricted to even I but we discuss odd I in section 7.) Although each solution is given uniquely by the set of labels λ, I, l, it is sometimes convenient to use the step-number $n_- = (I/2 - \lambda + 3l)/2$, defined above, in place of λ.

As first pointed out by Bès [1], it is also worth noting that each solution has a definite 'parity' corresponding to the operation $\gamma \to \gamma - \pi$. Then, ϕ_+ has odd parity while ϕ_0 is even. Both ladder operators have odd parity which enables us to deduce from the figure that the parity of each solution λ is given simply by $(-1)^\lambda$. The parity argument also implies that the coefficients $g(x)$, to be introduced in (18), have definite parity $(-1)^{l-b}$. This symmetry goes beyond the Octahedral group symmetry of the coordinates, discussed in section 2.1 and is due to the invariance of the ∇^2 operator with respect to the operation $\gamma \to \gamma - \pi$.

2.4. A triangular relation

The two ladder operators (5) and (6) may simply be combined to provide a 'triangular relation' between solutions. This will be helpful in obtaining a general solution from some particular cases, which are simpler. Subtracting (6) from (5) and using (11) gives

$$Y_{\lambda-1Il} = Y_{\lambda+1Il} + (2\lambda + 3)\phi_+ Y_{\lambda I-2l}. \tag{15}$$

We call this a triangular relation because it relates three solutions at the corners of a small triangle (with apex downward) in figure 1. In this expression, the values of λ are larger on the right than on the left. Hence, by repeated application, any solution may be written as a sum over solutions on the right-hand edge (which we call the 'top band' and corresponds to $n_- = 0$) of the rectangle in figure 1 defined by some fixed l. On this top band, the values of λ and I are related by $\lambda = 3l + I/2$. After some algebraic reduction, we find

$$Y_{\lambda Il} = \sum_k \binom{(3l + I/2 - \lambda)/2}{(I/2 - k)} \frac{(3l + I/2 + \lambda + 3)!!}{(3l - I/2 + \lambda + 2k + 3)!!} \phi_+^{I/2-k} Y_{3l+k2kl} \tag{16}$$

which expresses a general solution as a sum over solutions on the top band. The first factor on the right is a binomial coefficient and its upper argument is just n_- defined in section 2.3. The summation index k therefore runs over the $n_- + 1$ values from $I/2 - n_-$ to $I/2$.

3. Recurrence relations and explicit solutions in the ϕ_+, ϕ_0 basis

We now use the ladder operator (6) to derive explicit formulae for the $Y_{\lambda Il}$ on the top band by deriving a recurrence relation for the coefficients in the expansion in a complete set of basis functions constructed from the building blocks in equation (4). For a given I we need a product of $I/2$ of these blocks, and for convenience we introduce the symbol $n = I/2$, so that the basis functions, distinguished by a label b, are denoted

$$(\phi_+)^{n-b}(\phi_0)^b \tag{17}$$

with

$$Y_{\lambda Il} = \sum_{b=0}^{l} g_b^{\lambda Il}(x)(\phi_+)^{n-b}(\phi_0)^b \tag{18}$$

where $x = \cos 3\gamma$. Equations (11) to (14) show that an increase in the number of factors ϕ_0 in (17) occurs only from the differentiation $\partial/\partial x$. Hence, because the ladder process starts from a polynomial $P_l(x)$ of order l, the number b of such factors cannot exceed l. This justifies the upper limit for the sum in (18) and the vector space (17) has dimension $l + 1$.

From equations (11) to (14) we see that

$$\beta\partial/\partial a_{-2}(\phi_+)^{n-b}(\phi_0)^b = -(n + b)(\phi_+)^{n-b+1}(\phi_0)^b \tag{19}$$

and

$$\beta\partial g(x)/\partial a_{-2} = -3(x\phi_+ - \phi_0)\partial g(x)/\partial x. \tag{20}$$

Then, combining equations (6) and (18), using equations (19) and (20) and equating coefficients of a particular component $(\phi_+)^{n-b}(\phi_0)^b$ leads to the recurrence relation

$$g_b^{\lambda+1 I+2l} = -(\lambda + 3 + n + b + 3x\partial/\partial x)g_b^{\lambda Il} + 3\frac{\partial}{\partial x}g_{b-1}^{\lambda Il} \tag{21}$$

for the coefficients in the expansion of $Y_{\lambda+1\, I+2l}$ in terms of those of $Y_{\lambda Il}$. As explained in section 2.2, the solution for $I = 0$ is a Legendre polynomial $P_l(x)$. For other $Y_{\lambda Il}$ we therefore expand the coefficients in (18) as a power series

$$g_b^{\lambda Il}(x) = \sum_{\alpha=0}^{[(l-b)/2]} c_{b\alpha}^{\lambda Il} x^{l-b-2\alpha}. \tag{22}$$

The restriction here to a polynomial of order $l - b$ follows from the discussion given after equation (18). The square bracket in the upper limit to the sum denotes the 'integer part of' $(l - b)/2$.

Substituting into equation (21) and equating coefficients of each power gives the recurrence relation

$$c_{b\alpha}^{\lambda+1 I+2l} = -(\lambda + 3 + 3l - 2b - 6\alpha + n)c_{b\alpha}^{\lambda Il} + 3(l + 1 - b - 2\alpha)c_{b-1\alpha}^{\lambda Il}. \tag{23}$$

In the particular case of the top band, the variables λ and I are related by $\lambda = 3l + I/2$ and the recurrence relation simplifies to

$$c_{b\alpha}^{\lambda+1 l} = -(2\lambda + 3 - 2b - 6\alpha)c_{b\alpha}^{\lambda l} + 3(l + 1 - b - 2\alpha)c_{b-1\alpha}^{\lambda l} \tag{24}$$

where we have dropped the redundant I-label.

An important feature of this relation is that it involves no coupling between one value of α and another. For each α it may be applied repeatedly until λ has reduced back to its smallest value of $3l$ at $I = 0$ where the solution is the Legendre polynomial with

$$c_{0\alpha}^{3ll} = (-1)^\alpha \frac{(2l - 2\alpha)!}{2^l \alpha!(l - \alpha)!(l - 2\alpha)!}. \tag{25}$$

For any solution on the top band, labelled by the number of steps $k = \lambda - 3l$ from the starting point $I = 0$, we find that (24) has the solution

$$c_{b\alpha}^{3l+kl} = \frac{(-1)^{\alpha+b+k}(2l - 2\alpha)!3^b(6l - 6\alpha + 2k - 2b + 1)!!}{2^l\alpha!(l - \alpha)!(l - b - 2\alpha)!(6l - 6\alpha + 1)!!}\binom{k}{b}. \tag{26}$$

Finally, we insert this into the triangular relation (16) to obtain the completely general result

$$c_{b\alpha}^{\lambda Il} = \left[\frac{(-1)^{\alpha+b}3^b(2l - 2\alpha)!(3l + n + \lambda + 3)!!}{2^l\alpha!(l - \alpha)!(l - b - 2\alpha)!(6l - 6\alpha + 1)!!}\right]\sum_k (-1)^k\binom{k}{b}\binom{(3l + n - \lambda)/2}{n - k} \times \frac{(6l - 6\alpha + 2k - 2b + 1)!!}{(3l - n + \lambda + 2k + 3)!!}. \tag{27}$$

The form of the sum in equation (27) differs from that given earlier by Chacón *et al* [3] but can be shown to be equivalent. These authors use μ for the additional label, rather than the l in this paper, but, if we use the formula $\mu = (\lambda - l - n)/2 = l - n_-$ to relate these labels, our expression (27) for the coefficients in (22) can be shown to agree with [3] apart from an unimportant extra factor

$$(-1)^{(\lambda-3l+n)/2}(2\lambda + 1)!!/(\lambda + 3l - n + 1)!!$$

which amounts only to a different choice of normalization for the solutions. Our normalization is defined by the original Legendre polynomial at $I = 0$ and the ladder operators Q_+, Q_-. (We note that Frank and Van Isacker [5] use the symbol n_Δ for μ.) Solutions with some fixed μ

may therefore come from families of different l. Within a family of given l, the label μ runs over the interval $0 \leqslant \mu \leqslant l$, as shown in figure 1. Solutions with $\mu = l$ are on the top band while at the other extreme $\mu = 0$, the solutions lie on the parallel line starting from $I = \lambda = 2l$ which defines the left-hand limit of the l-rectangle. It is interesting that the sum in (27) is proportional to a hypergeometric function of type ${}_3F_2$ with argument unity. This is also true of the sum in [3] and the two sums are related through one of the various symmetries of these hypergeometric functions.

4. An alternative basis, ϕ_+, ϕ_-

Although the solution for $I = 0$ is a single Legendre polynomial, it was generally necessary, in the previous section, to revert to a power series in $\cos 3\gamma$, with formula (27) for the coefficients. In this section we show how the use of an alternative basis to (4) leads to general solutions in which the coefficients are expressed in terms of Legendre functions. For small I, very few coefficients are needed, providing a natural extension to the simple result for $I = 0$. Furthermore, we make use of 'angular-momentum' operators relating to the parameter l, which labels each family of solutions, and all the Legendre functions within that family carry the same l.

4.1. Recurrence relations and explicit solutions

As a basis we use ϕ_+ from (4) but, instead of ϕ_0, we take for the second member,

$$\phi_- = \mathrm{e}^{-\mathrm{i}\psi}(\sin\gamma\,\Phi_{220} - \cos\gamma\,\Phi_{222}) \tag{28}$$

which is related to the earlier pair (4) by $\sin 3\gamma\,\phi_- = \mathrm{e}^{-\mathrm{i}\psi}(\phi_0 - \cos 3\gamma\phi_+)$. Unlike ϕ_+ and ϕ_0 this new second member is not invariant under the Octahedral group but transforms according to the representation A_2. To restore the required Octahedral invariance it must always be multiplied by an odd power of $\sin 3\gamma$ but that will occur naturally in the coefficients to be determined. In fact these powers of $\sin 3\gamma$ are an essential part of the associated Legendre functions. We also note that ϕ_- is odd with respect to the Bès parity discussed at the end of section 2.3.

The role of the new variable ψ in (28) is a minor one which will become clear later. We need only to derive solutions for the top band since the triangular relation (16), being independent of basis, may again be used to generalize the results. For any solution on the top band we therefore expand, with the abbreviation $n = I/2$ again,

$$Y_{3l+nIl} = \sum_b f_b^{nl}(x,\psi)\phi_+^{n-b}\phi_-^b. \tag{29}$$

Since Y is to be independent of ψ, the function $f_b{}^{nl}$ must depend on ψ through the simple factor $\mathrm{e}^{\mathrm{i}b\psi}$. The task now is to use the ladder operators to obtain a recurrence relation for the $f_b{}^{nl}$, as functions of $x = \cos 3\gamma$, and to solve it.

Equations (12) and (14) must first be written in terms of the new basis vector ϕ_-

$$\beta\partial(\cos 3\gamma)/\partial a_{-2} = 3\mathrm{e}^{\mathrm{i}\psi}\sin 3\gamma\phi_- \tag{30}$$

$$\beta\partial\phi_-/\partial a_{-2} = -5\phi_+\phi_- - \mathrm{e}^{-\mathrm{i}\psi}\cot 3\gamma\left(\phi_+^2 - 3\mathrm{e}^{2\mathrm{i}\psi}\phi_-^2\right) \tag{31}$$

to give

$$\beta\partial\left\{f_b^{nl}\phi_+^{n-b}\phi_-^b\right\}/\partial a_{-2} = -(n+4b)f_b^{nl}\phi_+^{n-b+1}\phi_-^b + 3\mathrm{e}^{\mathrm{i}\psi}(\sin 3\gamma\,\partial/\partial\cos 3\gamma + b\cot 3\gamma)f_b^{nl}\phi_+^{n-b}\phi_-^{b+1} - b\,\mathrm{e}^{-\mathrm{i}\psi}\cot 3\gamma\,f_b^{nl}\phi_+^{n-b+2}\phi_-^{b-1}. \tag{32}$$

We now introduce, in a mathematical sense, the 'angular-momentum' operators, with 3γ and ψ as polar angles, which act only on the functions f and not on the basis vectors, defining in the usual way

$$L_{\pm} = \mp e^{\pm i\psi}(\sin 3\gamma\, \partial/\partial \cos 3\gamma \mp i \cot 3\gamma\, \partial/\partial\psi), \qquad L_0 = -i\partial/\partial\psi \tag{33}$$

and noting that, from the definition of f_b^{nl},

$$L_0 f_b^{nl} = -i\partial f_b^{nl}/\partial\psi = b f_b^{nl}. \tag{34}$$

Inserting this notation into (32) and using definition (6) of the ladder operator gives

$$\begin{aligned} Q_+\{f_b^{nl}\phi_+^{n-b}\phi_-^b\} &= -(3l+2n+3+4L_0)f_b^{nl}\phi_+^{n-b+1}\phi_-^b - 3L_+ f_b^{nl}\phi_+^{n-b}\phi_-^{b+1} \\ &\quad + \tfrac{1}{2}(e^{-2i\psi}L_+ + L_-)f_b^{nl}\phi_+^{n-b+2}\phi_-^{b-1}. \end{aligned} \tag{35}$$

In this expression, f is a function of the two polar angles 3γ and ψ while all other dependence on the variable $x = \cos 3\gamma$ is contained entirely in the angular-momentum operators. The dependence of f on ψ is trivial, namely that, see (34), f_b has 'magnetic quantum number' b. In using this equation we may therefore make use of the familiar algebra of angular momentum. Although spherical harmonics are commonly used in this algebra we prefer to use the un-normalized harmonics

$$Z_l^m = e^{im\psi} P_l^m. \tag{36}$$

The angular-momentum step operators are then simply

$$L_+ Z_l^m = -Z_l^{m+1}, \qquad L_- Z_l^m = -(l+m)(l-m+1)Z_l^{m-1}. \tag{37}$$

Since, in (35), the ladder operator is expressed in terms of the L-operators and the ladder process starts from $Y_{3l\,0l} = f_0^{0l} = Z_l^0 = P_l$ it is strongly suggested that $f_b{}^{nl}$ will be given simply in terms of the Legendre functions, noting (37). This is illustrated by some results obtained directly for one, two and three ladder steps (35) along the top band, starting from $I = 0$, and corresponding to $I = 2$ with $\lambda = 3l + 1$, $I = 4$ with $\lambda = 3l + 2$ and $I = 6$ with $\lambda = 3l + 3$ respectively,

$$\begin{aligned} Y_{3l+1\,2l} &= -3(l+1)P_l\varphi_+ + 3e^{i\psi}P_l^1\phi_- \\ Y_{3l+2\,4l} &= \left\{\tfrac{15}{2}(l+1)(l+2)P_l - \tfrac{3}{2}P_l^2\right\}\phi_+^2 - 18(l+2)\,e^{i\psi}P_l^1\phi_+\phi_- + 9e^{2i\psi}P_l^2\phi_-^2 \\ Y_{3l+3\,6l} &= \left[-\tfrac{3}{2}(l+1)(l+2)\{9(l+3)+8\}P_l + \tfrac{3}{2}\{9(l+3)-8\}P_l^2\right]\phi_+^3 \\ &\quad + \tfrac{27}{4}\{11(l+2)(l+3)P_l^1 - P_l^3\}\,e^{i\psi}\phi_+^2\phi_- - \\ &\quad - 81(l+3)\,e^{2i\psi}P_l^2\phi_+\phi_-^2 + 27P_l^3\,e^{3i\psi}\phi_-^3. \end{aligned} \tag{38}$$

Note that, although the new variable appears in these expressions, it is always accompanied by the appropriate power of ϕ_- to make Y independent of ψ overall.

Although it is straightforward to continue the ladder operations in this way to any I, it is clearly desirable to find a general solution. This is done by first acting with the ladder operator on (29), using (35) and equating coefficients of each basis vector to give the recurrence relation for the functions f as

$$f_b^{n+1\,l} = -(3l+2n+3+4L_0)f_b^{nl} - 3L_+ f_{b-1}^{nl} + \tfrac{1}{2}(e^{-2i\psi}L_+ + L_-)f_{b+1}^{nl}. \tag{39}$$

Examples (38) suggest using a Legendre expansion for f in the general case and we write

$$f_b^{nl} = \sum_{r=0}^{[\frac{1}{2}(n-b)]} 3^n\left(-\frac{1}{12}\right)^r \binom{b+r}{b}\rho(b,r)A_l(n,b,r)\,e^{-2ir\psi}Z_l^{b+2r} \tag{40}$$

where the exponential factor ensures that f has the correct dependence on ψ and the factor preceding the coefficient A is chosen, with hindsight, to make A simpler, as we shall see.

To avoid ambiguity, we have defined $\rho(b, r) = (b + 2r)/(b + r)$ with $\rho(0, 0) = 1$. Inserting (40) into (39) and equating to zero the coefficient of each spherical harmonic Z_l^{b+2r} leads to the recurrence relation

$$\begin{aligned}3(b+2r)A_l(n+1,b,r) &= -(3l+2n+3+4b)(b+2r)A_l(n,b,r)+3bA_l(n,b-1,r)\\&\quad+6rA_l(n,b+1,r-1)-\tfrac{1}{2}(b+r)(l+b+2r+1)(l-b-2r)A_l(n,b+1,r)\\&\quad+\tfrac{1}{4}b(l+b+2r+1)(l-b-2r)A_l(n,b-1,r+1)\end{aligned}\tag{41}$$

for the coefficients A. Inspection of this equation shows there to be a solution in the form of a polynomial of order $(n - b - 2r)$ in l but, rather than using a power series, we use the factorial series

$$A_l(n,b,r) = \sum_{i=0}^{n-b-2r} \frac{(l+n-i)!}{(l+b+2r)!} B_i(n,b,r).\tag{42}$$

This expansion is next substituted into (41) and the factors in (41) involving l may be absorbed into the series by writing, for example, $(l - b - 2r) = (l + n - i + 1) - (b + 2r + n - i + 1)$. Equating the coefficients of each factorial $(l + n - i)!$ on both sides of the equation gives the following equation for the B_i which are independent of l

$$\begin{aligned}(b+2r)B_{i+1}(n+1,b,r) &= -(b+2r)B_{i+1}(n,b,r)-\tfrac{1}{3}(b+2r)(3i+4b-n)B_i(n,b,r)\\&\quad+b\{B_{i+1}(n,b-1,r)-(n-b-2r-i+1)B_i(n,b-1,r)\}\\&\quad+2r\{B_{i+1}(n,b+1,r-1)-(n-b-2r-i+1)B_i(n,b-1,r)\}\\&\quad-\tfrac{1}{6}(b+r)\{B_{i+1}(n,b+1,r)-(n+b+2r-i+1)B_i(n,b+1,r)\}\\&\quad+\tfrac{1}{12}b\{B_{i+1}(n,b-1,r+1)-(n+b+2r-i+1)B_i(n,b-1,r+1)\}.\end{aligned}\tag{43}$$

Having extracted the dependence on $\cos 3\gamma$ in expansion (40) and the dependence on l in equation (42) it remains to solve (43) for the numerical coefficients B_i. Although this is a formidable recurrence equation it is not difficult to solve for small values of $i = 0, 1, 2$ and from these cases we guessed the general solution

$$\begin{aligned}B_i(n,b,r) &= (-1)^{n+b}\left(-\frac{8}{9}\right)^i \frac{n!}{i!}\\&\quad\times\sum_t\left(-\frac{1}{12}\right)^t \frac{(t+r)!}{(n-b-i-2r-2t)!(b+2r+t)!(t+r-i)!t!}.\end{aligned}\tag{44}$$

In practice, the number of allowed values of i is severely restricted by the constraint $i \leqslant [(n - b)/3]$ which results from the factorials in (44). The veracity of this solution was then confirmed by substitution into (43), see appendix B, and although it refers only to the top-band, the general solution may then be constructed by using the triangular relation (16) together with equations (29), (36) and (40) to give

$$Y_{\lambda I l} = \sum_{b=0}^{n} \sum_{r=0}^{[(n-b)/2]} a_{\lambda l}(n,b,r) P_l^{b+2r}(x)\phi_+^{n-b}(\mathrm{e}^{\mathrm{i}\psi}\phi_-)^b\tag{45}$$

where

$$\begin{aligned}a_{\lambda l}(n,b,r) &= 3^n\left(-\frac{1}{12}\right)^r\binom{b+r}{b}\rho(b,r)\sum_{w=0}^{n_-}\binom{n_-}{w}3^{-w}\\&\quad\times\frac{(6l+2n-2n_-+3)!!}{(6l+2n-2n_-+3-2w)!!}A_l(n-w,b,r)\end{aligned}\tag{46}$$

and where $n_- = (3l + n - \lambda)/2$ was introduced in section 2.3.

4.2. The reflection symmetry $l \to -(l+1)$

Within each family l there is an interesting 'reflection' symmetry corresponding to a change of sign of the quantity $(l+1/2)$ or, in other words the operation $l \to -(l+1)$. This reflection, which has its origin in the Legendre functions, has been discussed for the group $O(3)$ in the context of negative angular momentum, by Biedenharn and Louck [6] and others. In the present context, we find that the solutions Y_{3l+kIl} and Y_{3l-kIl} are related by carrying out this operation on the coefficients $A(n, b, r)$ in expansion (40). In particular, the solutions Y_{3lIl} depend only on the invariant $l(l+1)$. For example, in comparison with (38)

$$Y_{3l-1\,2l} = 3l P_l \phi_+ + 3\mathrm{e}^{\mathrm{i}\psi} P_l^1 \phi_-$$

while

$$Y_{3l\,4l} = \left\{-\tfrac{21}{2} l(l+1) P_l - \tfrac{3}{2} P_l^2\right\}\phi_+^2 - 21 P_l^1\, \mathrm{e}^{\mathrm{i}\psi} \phi_+\phi_- + 9 P_l^2\, \mathrm{e}^{2\mathrm{i}\psi} \phi_-^2. \tag{47}$$

The origin of this symmetry lies in the ladder operators (5) (6) in which the step-up and step-down operators differ only in the operation $\lambda \to -(\lambda+3)$. In other words,

$$Q_+(3l-k) = Q_-(-3l-3+k) \tag{48}$$

which contains the reflection described above and the change of sign for k. The general result then follows from this symmetry in each step as the two solutions Y_{3l+kIl} and Y_{3l-kIl} are constructed from $I = 0$. Although the second term in (5) and (6) gives rise to some l-dependence when acting on the Legendre functions, the contribution is invariant under the reflection, see (37). This symmetry applies to all solutions for $I \leqslant 2l$ but for greater $2l \leqslant I \leqslant 4l$ it is relevant only for $\lambda \leqslant 5l - I/2$. For values of λ beyond this range the reflected image with smaller λ falls outside the rectangle defining l and no such solution exists. This reflection symmetry is not apparent when using the basis ϕ_+, ϕ_0 in section 3.

4.3. The calculation of matrix elements and norms

The calculation of matrix elements of physical operators, including norms, in the wavefunctions $Y_{\lambda Il}$ involves integration over both γ and the three Euler angles Ω and this problem has been discussed in some detail in earlier papers [3] and in the book of Eisenberg and Greiner [7], using the basis ϕ_+, ϕ_0. We now indicate how the problem simplifies in the new basis ϕ_+, ϕ_- because of the separation of the γ and Ω variables.

The general solution (45) is given by

$$Y_{\lambda Il} = \sum_{b=0}^{n} \sum_{r=0}^{[(n-b)/2]} a_{\lambda I}(n, b, r) P_l^{b+2r}(x)|b\rangle \tag{49}$$

where $|b\rangle$ denotes the basis element $\phi_+^{n-b}(\mathrm{e}^{\mathrm{i}\psi}\phi_-)^b$ and the coefficient $a_{\lambda I}(n, b, r)$ was given in equation (46). (Note that the angle ψ is completely absent in this form.) The Ω-dependence lies only in the basis element whereas γ is present both in the Legendre functions and in the basis. A succession of three simple transformations reduces $|b\rangle$ to a sum over the rotation matrices $D^I_{IK}(\Omega)$, enabling the Ω-integration to be done and, at the same time, separates out the dependence on γ. We first introduce

$$\Phi = (\Phi_{220} + \mathrm{i}\Phi_{222})/\sqrt{2} \qquad \text{and} \qquad \bar{\Phi} = (\Phi_{220} - \mathrm{i}\Phi_{222})/\sqrt{2} \tag{50}$$

so that

$$\phi_+ = (\mathrm{e}^{-\mathrm{i}\gamma}\Phi + \mathrm{e}^{\mathrm{i}\gamma}\bar{\Phi})/\sqrt{2}, \qquad \mathrm{e}^{\mathrm{i}\psi}\phi_- = \mathrm{i}(\mathrm{e}^{-\mathrm{i}\gamma}\Phi - \mathrm{e}^{\mathrm{i}\gamma}\bar{\Phi})/\sqrt{2} \tag{51}$$

and, by expanding the two binomials, we have

$$|b\rangle = 2^{-n/2} i^b \sum_{y=0}^{n} G(n,b,y)\Phi^{n-y}\bar{\Phi}^y \,\mathrm{e}^{\mathrm{i}\gamma(2y-n)} \tag{52}$$

where $G(n,b,y) = \sum_r (-1)^{b-r}\binom{b}{r}\binom{n-b}{n-y-r}$ is proportional to a Jacobi polynomial at zero argument and also to a reduced rotation matrix $d^{n/2}(\pi/2)$, see Biedenharn [6].

This separates out the γ-dependence into a single exponential and, with a similar expansion of binomials, the Ω-dependent factor becomes

$$\Phi^{n-y}\bar{\Phi}^y = 2^{-n/2}\sum_z i^z G(n,y,z)\Phi_{220}^{n-z}\Phi_{222}^z. \tag{53}$$

The products in (53) may then be reduced, using properties of the rotation matrices, to the sum

$$\Phi_{220}^{n-z}\Phi_{222}^z = \sum_{K\geqslant 0} 2^{(n-2z+1)/2}3^{(n-z)/2}\sqrt{\frac{(2n+K)!(2n-K)!}{(4n)!(1+\delta_{K,0})}}\frac{z!}{\left(\frac{1}{2}z+\frac{1}{4}K\right)!\left(\frac{1}{2}z-\frac{1}{4}K\right)!}\Phi_{IIK} \tag{54}$$

where the Φ_{IIK} were defined in equation (2). The sum over K is naturally restricted to $K = 0, 4, 8, \ldots$ for even z and to $K = 2, 6, 10, \ldots$ for odd z. The Ω-dependence is now entirely contained in the Φ_{IIK} which are orthogonal on K with standard norm $8\pi^2/(2I+1)$ so that the integral over Ω is simply carried out, depending on the Ω-dependence of the operator whose matrix element is being calculated. The γ-integrals contain a product of Legendre functions from (49) together with the exponential from (52) and any other factor from the operator. Because of the Octahedral symmetry of the coordinates, discussed in section 2.1, the contributions from some relative values $(y'-y)$ of y between bra and ket are zero. For example in calculating the norm, this difference must be a multiple of 3 because the integrand has to be an invariant, which implies being a function only of the multiple 3γ. Hence the γ-integrals in the norm are of the sort

$$\int_0^{\pi/3} P_l^m(x)P_{l'}^{m'}(x)\,\mathrm{e}^{6\mathrm{i}p\gamma}\sin 3\gamma\,\mathrm{d}\gamma \tag{55}$$

where p is an integer and these can be expressed in terms of the integrals

$$\int_{-1}^{1} P_l^m P_{l'}^{m'}(1-x^2)^a\,\mathrm{d}x = (-1)^{(l-l'-m+m')/2}2^{2a+l-l'+1}\frac{(l'+m')!}{(l-m)!\left[\frac{l'+m'}{2}\right]!\left[\frac{l'-m'}{2}\right]!}$$
$$\times\sum_{r=0}\left(-\frac{1}{2}\right)^r r!(2l-2r-1)!!\binom{\left[\frac{l-m}{2}\right]}{r}\binom{\left[\frac{l+m}{2}\right]}{r}$$
$$\times\frac{\left(a+\left[\frac{l+m'}{2}\right]-r\right)!\left(a+\left[\frac{l-m'}{2}\right]-r\right)!}{(2a+l-l'-2r)!!(2a+l+l'+1-2r)!!}. \tag{56}$$

Expression (56) is valid if $a\geqslant 0$ and $2a+l-l'$ is a positive even integer. It was obtained by using various properties of the Legendre functions and is non-zero only for even values of $(l+l'+m+m')$. The square brackets again denote the integer part and are necessary to distinguish between even and odd values of, for example, $(l+m)$. Without loss of generality, we take $m\geqslant m'$ whereupon the range of the summation index r is restricted to $r\leqslant a+(l-l')/2$. For example when $a=0$ and $l=l'$ there is only one term $r=0$ and the integral is simply

$$(-1)^{(m-m')/2}\frac{2(l+m')!}{(2l+1)(l-m)!}. \tag{57}$$

In practice, for calculating norms and overlaps when $I < 12$, the only values of p which occur are $p = 0$ or $p = 1$ and, as l and l' differ by 2 at most, the maximum value of r in (56) is 2. We give the norms and overlaps for $I \leqslant 8$ in appendix C. Although they were calculated using solution (46) these norms and overlaps are also valid for solution (27) in the basis ϕ_+, ϕ_0 used in section 3. This follows because the same ladder procedure (5), (6) was used to define the solutions in each case.

4.4. The Octahedral group structure of the solutions

In section 2.1 we explained that the solutions must be invariant under the Octahedral group and this is apparent from equation (49) in which both the Legendre function and the basis vector $|b\rangle$ transform according to the invariant representation A_1 if b is even and according to the other one-dimensional representation A_2 if b is odd. However, the symmetry of the separate γ and Ω components of $|b\rangle$ is lost in the reduction to the convenient basis Φ_{IlK} through equations (52), (53) and (54). In this section we show how to write the general solution in terms of separate γ and Ω factors which transform irreducibly.

The first step is to rewrite (52) as

$$\begin{aligned}|b(\text{even})\rangle &= 2^{-n/2}(-1)^{b/2}\sum_{y=0}^{[n/2]} G(n,b,y)\{\cos(n-2y)\gamma|y^+) + \sin(n-2y)\gamma|y^-)\}\\ |b(\text{odd})\rangle &= 2^{-n/2}(-1)^{(b-1)/2}\sum_{y=0}^{[n/2]} G(n,b,y)\{\sin(n-2y)\gamma|y^+) - \cos(n-2y)\gamma|y^-)\}\end{aligned} \tag{58}$$

where we have used the relation $G(n, b, n-y) = (-1)^b G(n, b, y)$, thereby halving the range of the y-sum, and the round-bracket kets denote the combinations

$$|y^+) = (\Phi^{n-y}\bar{\Phi}^y + \Phi^y\bar{\Phi}^{n-y})/(1+\delta_{n,2y}), \qquad |y^-) = (\Phi^{n-y}\bar{\Phi}^y - \Phi^y\bar{\Phi}^{n-y})/\text{i}. \tag{59}$$

The next step is to argue that $|y^+)$ and $|y^-)$ transform according to A_1 and A_2 respectively if $(n-2y)$ is a multiple of 3 and if not, that they transform according to the two components of the representation E. To show this we recall that the Octahedral group is generated by the two rotations $\Re_z(\pi/2)$ and $\Re_y(\pi/2)$, see [4]. For the one-dimensional representations both operators have a matrix element of +1 for A_1 and –1 for A_2. The representation E is typified by the functions Φ_{220} and Φ_{222} giving matrices

$$\Re_z(\pi/2) = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \Re_y(\pi/2) = \begin{pmatrix}-1 & \sqrt{3}\\ \sqrt{3} & 1\end{pmatrix}\Big/2 \tag{60a}$$

so that, in the basis $\Phi, \bar{\Phi}$ of (50), the matrices become

$$\Re_z(\pi/2) = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \Re_y(\pi/2) = \begin{pmatrix}0 & \text{e}^{-2\pi\text{i}/3}\\ \text{e}^{2\pi\text{i}/3} & 0\end{pmatrix} \tag{60b}$$

which gives

$$\begin{aligned}&\Re_z(\pi/2)|y^{\pm}) = \pm|y^{\pm})\\ &\Re_y(\pi/2)|y^{\pm}) = \pm\{\cos 2\pi(n-2y)/3|y^{\pm}) \pm \sin 2\pi(n-2y)/3|y^{\mp})\}.\end{aligned} \tag{61}$$

If $(n-2y) = 3p+1$ with p any integer, this shows that $|y^+)$ and $|y^-)$ transform precisely according to the representation E in the basis (60a). When $(n-2y) = 3p-1$ the same is true for $|y^+)$ and $-|y^-)$ and for the case $(n-2y) = 3p$, equation (61) shows that $|y^+)$ and $|y^-)$ transform like A_1 and A_2 respectively.

The geometry of the coordinates in five dimensions implies that the two generators in (60) lead to the transformations $\gamma \to -\gamma$ and $\gamma \to -\gamma + 2\pi/3$ respectively. It follows that the functions $\cos\gamma(2n - y)$ and $\sin\gamma(2n - y)$ transform in exactly the way that we have just described for $|y^+)$ and $|y^-)$. The combinations of these trigonometric functions with the $|y^+)$ and $|y^-)$ in (58) are then necessarily those which produce overall A_1 symmetry for even b and A_2 symmetry for odd b. (The coefficients in the combinations are essentially the Clebsch–Gordan coefficients for the Octahedral group, which are just $\pm 1/\sqrt{2}$ in these cases.)

We therefore have the result that (49) with (58) gives an expansion of $Y_{\lambda Il}$ in a basis $|y^{\pm})$ of functions of Ω which transform irreducibly under the Octahedral group, in place of the $D_{IK}{}^{I}(\Omega)$ in (54). These functions are not normalized and, when a particular representation occurs more than once for a given I, as it does for $I \geqslant 8$, they are not orthogonal. There is, of course, orthogonality between different representations and between the two components of the E-representation. We illustrate this form of solution in appendix E.

4.5. The introduction of 'spin' and its vector coupling to l to form j

In section 4.1 we introduced operators $\mathbf{L}$ to help in constructing the coefficients in an expansion of the solution in a basis formed of a product of $I/2$ factors of the building blocks ϕ_+ and ϕ_-. Here we regard these two functions as defining a spin-space with $s = 1/2$ so that the basis for an arbitrary I with dimension $I/2 + 1$, as used in section 4.1, will have spin $s = n/2 = I/4$. In principle, we may vector couple l and s in the usual way to form a resultant $\vec{j} = \vec{l} + \vec{s}$. If we choose a projection $\langle j_z\rangle = s$ then the range of j-values is given by $\min\{|l - s|, s\} \leqslant j \leqslant (l + s)$. If j is now connected to λ by the relation $\lambda = 2j + l$ this range of j-values translates into the range $\max\{3l - 2s, l + 2s\} \leqslant \lambda \leqslant 3l + 2s$ for λ. Comparison with figure 1 shows that this region is precisely the rectangle defining the family l. The upper limit is the top band and the two lower limits correspond to the band-heads and the other side of the rectangle, which is parallel to the top band. There is therefore a one-to-one correspondence between the range of solutions for given l and the usual range of j-values, given l, s and the projection $\langle j_z\rangle = s$.

The important question remains as to whether the vector-coupled wavefunctions have any connection to the detailed solutions constructed in section 4.1. For $I = 0$ there is nothing to be said because $s = 0$ and $l = j$ only. For $I = 2$, $s = 1/2$ so that $j = l \pm 1/2$ corresponding to $\lambda = 3l \pm 1$. We now show that the solutions derived earlier in these cases agree precisely with the corresponding vector-coupled wavefunctions.

In this case, the ladder operator Q_+ takes the simple form

$$\begin{aligned} Q_+(3l)P_l &= -(3l+3)P_l\phi_+ - 3L_+P_l\phi_- = -3\{(l+1) + L_+S_-\}P_l\phi_+ \\ &= -3\{(l+1) + 2(L.S)\}P_l\phi_+ \end{aligned} \tag{62}$$

where we have used $S_-\phi_+ = \phi_-$, and $S_+\phi_+ = 0$. The product $P_l\,\phi_+$ can only be a mixture of $j = l \pm 1/2$ but the operator on the right of (62) is the destruction operator for $j = l - 1/2$ because, trivially, the value of $2(L.S)$ is given by $j(j+1) - l(l+1) - s(s+1)$. Hence the ladder operator on the left of (62) must produce a state of pure $j = l + 1/2$. By a similar argument, Q_- produces $j = l - 1/2$. It may easily be confirmed that the coefficients for these two solutions, given in (38) and (47), agree with the conventional Clebsch–Gordan coefficients if the standard normalization is applied to the spherical harmonics Z in (36).

For $I > 2$ the third term on the right-hand side of (35) contributes to the ladder operators and, although it is still possible to use the label $j = (\lambda - l)/2$ there are increasingly complicated correction factors multiplying the Clebsch–Gordan coefficients and we have not pursued this avenue.

5. The limit of large λ and finite $I \ll \lambda$

In this section we consider large l, so that λ is also large while I remains finite and small compared with λ. For large l there is an asymptotic formula for the spherical harmonics, see [8], which is remarkably accurate and implies, for the Legendre functions, used in (36),

$$P_l^m(\cos 3\gamma) \approx (-1)^m \sqrt{\frac{2}{\pi \sin 3\gamma}} \left(l + \frac{1}{2}\right)^{m-\frac{1}{2}} \sin\left\{\left(l + \frac{1}{2}\right) 3\gamma + \left(m + \frac{1}{2}\right) \frac{\pi}{2}\right\}. \tag{63}$$

It is possible to extend the arguments of the previous section to large λ and make use of (63) to arrive, eventually, at some very simple results. We find that the solutions fall into three categories, depending on whether λ is divisible by 3, i.e. $\lambda = 3l$, or $\lambda = 3l \pm 1$. (This is the extension of the even–odd concept to the number 3.) For $\lambda = 3l$, there are generally two kinds of solution

$$Y = \sqrt{\frac{6}{\pi \sin 3\gamma}} \cos\left\{\gamma\left(\lambda + \frac{3}{2}\right) - \frac{\pi}{4}\right\} |A_1\rangle \tag{64}$$

$$Y = \sqrt{\frac{6}{\pi \sin 3\gamma}} \sin\left\{\gamma\left(\lambda + \frac{3}{2}\right) - \frac{\pi}{4}\right\} |A_2\rangle \tag{65}$$

and for $\lambda = 3l \pm 1$,

$$Y = \sqrt{\frac{3}{\pi \sin 3\gamma}} \left[\cos\left\{\gamma\left(\lambda + \frac{3}{2}\right) - \frac{\pi}{4}\right\} |E_1\rangle \pm \sin\left\{\gamma\left(\lambda + \frac{3}{2}\right) - \frac{\pi}{4}\right\} |E_2\rangle\right]. \tag{66}$$

The kets are the orthonormal Octahedral representations A_1, A_2 and E, see appendix E, which occur for each chosen I, usually given as a sum over the $D^I_{IK}(\Omega)$ and where E_1 and E_2 denote the two components of the representation E in the real basis transforming like Φ_{220} and Φ_{222}. The reduction of the $(2I+1)$-dimensional representation of the rotation group into Octahedral representations is described in appendix E. The volume element for the Euler angles is the usual $\mathrm{d}\Omega = \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi \,\mathrm{d}\psi$ and, for the γ-variable we use $\sin 3\gamma \,\mathrm{d}\gamma$ over the range 0 to $\pi/3$.

It is instructive to consider examples for small I making use of table 5. For $I = 0$, there is just one solution, which must be given by equation (64), with λ a multiple of 3. For $I = 2$, table 5 shows just the representation E so that equation (66) applies with $\lambda = 3l \pm 1$. For given λ there is only one solution because no λ can fall into both ± categories for integer l. The Octahedral representation E is, in this case, just the original basis Φ_{220}, Φ_{222} introduced in section 2.1. For $I = 4$, table 5 shows that there is an A_1 solution when $\lambda = 3l$ and E solutions when $\lambda = 3l \pm 1$. At $I = 6$, table 5 shows that there are both A_1 and A_2 type solutions when λ is a multiple of 3, together with an E representation when λ has the form $3l \pm 1$. When $I > 6$, some of the representations A_1, A_2 and E occur more than once in the reductions in table 5 and an arbitrary orthogonal basis will need to be constructed, as illustrated in table 6 for $I = 8$.

When l is finite, the general solutions (49) with (58) may always be expressed as a sum over different representations but for large l, only one is involved. In other words the coefficients of all representations but one go to zero for large l.

To understand the extreme simplicity of solutions (64) to (66) at large λ we return to the Casimir operator introduced in section 2.2 and its eigenvalue equation

$$\Lambda Y_{\lambda Il} = \left[-\frac{1}{\sin 3\gamma}\frac{\partial}{\partial\gamma}\left(\sin 3\gamma \frac{\partial}{\partial\gamma}\right) + T_{\mathrm{rot}}\right] Y_{\lambda Il} = \lambda(\lambda+3) Y_{\lambda Il} \tag{67}$$

where T_{rot} is the usual rotational energy, involving derivatives with respect to the Euler angles. By writting $Y_{\lambda Il} = Z_{\lambda Il}/\sqrt{\sin 3\gamma}$ the corresponding equation for Z becomes

$$\frac{\partial^2}{\partial\gamma^2}Z + \left[\left(\lambda + \frac{3}{2}\right)^2 + \frac{9}{4\sin^2 3\gamma} - T_{\mathrm{rot}}\right]Z = 0 \tag{68}$$

from which we see that, for large λ, the γ-dependence of Z must be some combination of $\cos\left(\lambda + \frac{3}{2}\right)\gamma$ and $\sin\left(\lambda + \frac{3}{2}\right)\gamma$, in agreement with the results in equations (64) to (66). The particular combinations in these equations can then be understood in terms of the overall Octahedral and Bès symmetries discussed in section 2.

6. *E*2 transitions

The simplest $E2$ operator in the five-dimensional problem is proportional to a_μ in the notation of equation (7) but we omit the 'radial' factor β since, in this paper, we are only concerned with the $O(5)$ variables. For a transition $I \to I-2$ it is only necessary to use the $\mu = 2$ component with the wavefunctions $Y_{\lambda Il}$ in this paper, which have $M = I$. In other words, the $E2$ operator is the ϕ_+ introduced in (4). This enables us to make use of the triangular relation (15) to relate the $E2$ matrix elements to the norms of the wavefunctions, as follows.

For brevity, write $Y_{\lambda Il} \equiv |\lambda Il\rangle$. Then, from (15) we have immediately

$$\langle\lambda \pm 1Il'|\phi_+|\lambda I-2l\rangle = \mp\left(\frac{1}{2\lambda+3}\right)\langle\lambda \pm 1Il|\lambda \pm 1Il\rangle. \tag{69}$$

Dividing by the norms of the two wavefunctions on the left gives

$$B(E2 : \lambda \pm 1Il' \to \lambda I-2l) = \left(\frac{1}{2\lambda+3}\right)^2 \frac{\langle\lambda \pm 1Il'|\lambda \pm 1Il\rangle^2}{\langle\lambda \pm 1Il'|\lambda \pm 1Il'\rangle\,\langle\lambda I-2l \mid \lambda I-2l\rangle} \tag{70}$$

and values can be read off from the norms and overlaps in tables 3 and 4 of appendix D. For the $I \to I$ transitions a direct calculation gives $B(E2\text{: } \lambda = 3l+2, l+1 \to \lambda = 3l+1, l) = 2/7$ for the only transition with $I = 2$, while, for $I = 4$ there are three types of transition with

$$B(E2 : 3l+2, l \to 3l+1, l+1) = 276l(l+2)/385(6l+3)(6l+7)$$
$$B(E2 : 3l+1, l+1 \to 3l, l) = 2(6l+1)(6l+7)/33(2l+1)(6l+5)$$
$$B(E2 : 3l, l \to 3l-1, l-1) = 2(6l-1)(6l+5)/33(2l+1)(6l+1).$$

In the limit of large λ, the simple solutions (64) to (66) lead to the closed formulae

$$B(E2 : \lambda = 3l \pm 1, EI \to \lambda = 3l \pm 2, EI') = (2I'+1)\left\{\sum_K c_K^{E_1 I} c_K^{E_1 I'} \begin{pmatrix} 2 I I' \\ 0 K -K \end{pmatrix}\right\}^2$$

$$B(E2 : \lambda = 3l, A_1 I \to \lambda = 3l \pm 1, EI') = \frac{1}{2}(2I'+1)\left\{\sum_K c_K^{A_1 I} c_K^{E_1 I'} \begin{pmatrix} 2 I I' \\ 0 K -K \end{pmatrix}\right\}^2$$

$$B(E2 : \lambda = 3l, A_2 I \to \lambda = 3l \pm 1, EI') = \frac{1}{2}(2I'+1)\left\{\sum_K c_K^{A_2 I} c_K^{E_1 I'} \begin{pmatrix} 2 I I' \\ 0 K -K \end{pmatrix}\right\}^2$$

which contain $3j$-symbols on the right, together with the expansion coefficients ${c_K}^{RI}$ for the Octahedral functions given in table 6 of appendix E for $I \leqslant 8$. It is soon verified that they agree with the general results above when $l \to \infty$.

It is also of interest to see how these very simple results for large l compare with the exact results above for finite l. Table 1 shows the ratios of $B(E2)$ values for some finite l to those at $l = \infty$ for some $I \to I-2$ transitions within the $n_- = 0$ and $n_- = 1$ bands.

Table 1. A comparison of some $B(E2)$-values between finite and infinite l.

n_-	I	$l=0$	1	2	3	4
0	2	2.00	1.33	1.20	1.14	1.11
0	4	2.40	1.64	1.41	1.30	1.24
0	6	2.60	1.86	1.58	1.44	1.36
1	4	–	2.10	1.57	1.38	1.29
1	6	–	2.36	1.79	1.55	1.43

7. Odd *I*

For most of this paper we have restricted the discussion to even values of I but results for odd I are simply related to those for even I, as we now show. From equation (2) it is clear that there is no solution for $I = 1$ and, as with the solutions for $I = 0$, the $I = 3$ solutions can be found directly from the Casimir operator. They are found to be

$$Y_{3(l+1)3l} = P^1_{l+1}(x)\Phi_{332} \tag{71}$$

with $\lambda = 3(l + 1)$ and $l = 0, 1, 2, \ldots$, where again we have chosen the maximum $M = 3$.

The ladder operators can then be used, as before, to construct the other solutions. For odd I, the pattern of solutions is therefore identical to figure 1 and may be superimposed onto figure 1 with its origin positioned at $\lambda = I = 3$ instead of $\lambda = I = 0$. Moreover, the values of the numbers n_+ and n_- introduced in section 2.3, are obtained by the replacements $\lambda - 3$ for λ and $I - 3$ for I in the expressions given for even I. It follows that, for odd I, the range of values for I and l is obtained by making these replacements in the previous formulae. In particular, for given λ and l, the range of I is given by

$$2|\lambda - 3l - 3| + 3 \leqslant I \leqslant 2\lambda - 2l - 3$$

where I moves in steps of 4. This shows that for $l = 0$, there is a single odd solution for each $\lambda \geqslant 3$ with $I = 2\lambda - 3$ analogous to the band of even solutions with $I = 2\lambda$. For the remainder of this section we will reserve the symbol I for the odd solutions and, as an aid to clarity, use the abbreviation $I_E = I - 3$ for the corresponding even solutions.

To find detailed solutions for odd I, we make use of the operator

$$V = -\frac{1}{3}\left(a_1\frac{\partial}{\partial a_{-2}} + a_2\frac{\partial}{\partial a_{-1}}\right) \propto (a \times \nabla)^3_3$$

which is a generator of the $O(5)$ group. It follows immediately that V, acting on a solution with even I_E and $M = I_E$, produces a solution of the same λ with $I = I_E + 3$ and $M = I$. We may therefore define the solution for any odd $I \geqslant 3$ by

$$Y_{\lambda Il} = VY_{\lambda I_E l+1}. \tag{72}$$

This prescription is especially simple to apply in the ϕ_+, ϕ_0 basis of section 3, as $V\phi_+ = V\phi_0 = 0$. Moreover, from equations (9) and (10), $V\beta = 0$ and $V\gamma = -\Phi_{332}/3$ so that, in the notation of (18),

$$g_b^{\lambda Il}(x) = Vg_b^{\lambda I-3l+1}(x) = \sin 3\gamma \frac{\mathrm{d}}{\mathrm{d}x} g_b^{\lambda I-3l+1}(x)\Phi_{332}. \tag{73}$$

In other words, the solution for odd I in this basis is obtained by differentiating the coefficient in the solution for the corresponding even $I_E = I - 3$ and inserting a factor $\sin 3\gamma\ \Phi_{332}$. This is a simple operation because g is given as a power series (22). Equation (71) is a special case of this. It is worth noting that odd states defined by (72) also satisfy the triangular relation, equation (15).

The application of equation (72) is different in the ϕ_+, ϕ_- basis of section 4 because V does not give zero when acting on ϕ_-. Instead,

$$V\phi_- = (\cos 3\gamma\phi_- - \sin 3\gamma\phi_+ \,\mathrm{e}^{-\mathrm{i}\psi})\Phi_{332}/\sin 3\gamma. \tag{74}$$

In analogy with equation (45) we again write the solutions in terms of Legendre functions,

$$Y_{\lambda Il} = \sum_{b=0}^{n} \sum_{r=0}^{[(n-b)/2]} \tilde{a}_{\lambda l}(n, b, r) P_{l+1}^{b+2r+1}(x)\phi_+^{n-b}(\mathrm{e}^{\mathrm{i}\psi}\phi_-)^b \Phi_{332} \tag{75}$$

where $n = I_E/2$ and we describe two independent ways in which the coefficients $\tilde{a}_{\lambda l}(n, b, r)$ may be related to previous results for the even solutions. Using (72) and (74), we find the relation

$$\tilde{a}_{\lambda l}(n, b, r) = \frac{a_{\lambda l+1}(n, b, r)}{\rho(b, r)} - (b+1)a_{\lambda l+1}(n, b+1, r) - \frac{(r+1)(l+b+2r+3)(l-b-2r)}{(b+r+2)} a_{\lambda l+1}(n, b, r+1) \tag{76}$$

where $\rho(b, r)$ was defined just after equation (46). This gives the coefficients for given λ and odd I as simple combinations of those of the corresponding even solution with the same λ.

Consider as an example the $I = 7$ top-band solutions with $\lambda = 3l + 5$. Using the entries for $I = 4$, $n_- = 0$ from table 2 in appendix C, replacing l by $l + 1$ and substituting into equation (76) gives, for any $l \geqslant 0$

$$\tilde{a}_{3l+5l}(2, 0, 0) = 33(l+3)(l+4)/4, \qquad \tilde{a}_{3l+5l}(2, 1, 0) = -18(l+4),$$
$$\tilde{a}_{3l+5l}(2, 2, 0) = 9, \qquad \tilde{a}_{3l+5l}(2, 0, 1) = -3/4.$$

Reflection symmetry again provides solutions when n_- is replaced by $n - n_-$ but the symmetry operation is now $l \to -(l+3)$.

As an alternative to the use of (76) we have followed through the arguments of section 4, but with I odd rather than even. This shows that the $\tilde{a}_{\lambda l}(n, b, r)$ are again given by equation (46), but with the following changes:

(i) Add 1 to b and l throughout and to $(n - w)$ in the function A.
(ii) Include an extra factor $(b + 1)/(n - w + 1)$.

8. Summary

We introduced simple ladder operators in section 2 which step from a solution λI to one with $\lambda \pm 1\ I + 2$. This enables the generation of the full array of solutions shown in figure 1, starting from $I = 0$ for which the solutions are simply the Legendre polynomials $P_l\ (x)$ with $x = \cos 3\gamma$. The array is thus divided into families labelled by l. Section 3 reproduced earlier results [3] by a more direct method, by first deriving and solving a simple recurrence relation for a sub-set of solutions, the 'top band' with $\lambda = 3l + I/2$, and then using a triangular relation, derived in section 2.4, to get the general solution.

Section 4 introduced a new basis for the Euler angle dependence of the solution leading to an alternative form for the solutions involving relatively few associated Legendre functions $P_l^m\ (x)$ rather than power series as in [3]. (Although Gheorghe [9] expressed the solutions as a series of Gegenbauer polynomials, which are closely related to the Legendre functions, his solutions differ from ours in two important respects; he uses the basis of section 3 rather than that of section 4 and also his sums run over many l-values while, here, each solution has a unique value of l.) A new reflection symmetry was noted in section 4.2, whereby one solution may be obtained directly from another. In section 4.4, the solutions were expressed in terms of representations of the underlying Octahedral symmetry group of the five-dimensional coordinates. We briefly investigated the introduction of a 'spin' defined by $s = I/4$ and, although, for $I = 2$, this led to solutions given precisely by the standard vector-coupling $\vec{l} + \vec{s} = \vec{j}$, this simplicity is lost for higher I. The label j may still be used but the coupling coefficients are no longer standard. However, in section 5 we used the spin concept to derive simple closed expressions for the solutions in the limit $\lambda \to \infty$ with I finite. The solutions fell into several classes, depending on whether λ is a multiple of 3 or a multiple of 3 plus or minus 1. The Euler- angle dependence is given, in each case, by a single Octahedral group representation.

Some $B(E2)$ values are calculated in section 6, which includes a comparison with the results at large λ, for which closed formulae are given. Although most of the paper is concerned with even I, it has been known for a long time that the extension to odd-I is straightforward and this is described briefly in section 7.

Appendix A. A restriction to the array of solutions

Here we justify the remark in section 2.3 that, in the procedure for constructing the array of solutions with given l, the lowering operator Q_- must not be applied more than l times. To do this we show that the $(l + 1)$th application of Q_- on the starting function $P_l(x)$ at $I = 0$ produces a solution lying in the vector space spanned by a set of solutions with smaller l. It is thus not independent of those solutions and should be discarded.

The solution obtained by $(l + 1)$ applications of the operator Q_- has $\lambda = 2l - 1$, $I = 2(l + 1)$ and is given by (17), (18), and (22) where formula (27) for the coefficient simplifies to

$$c_{b\alpha}^{2l-12(l+1)l} = \frac{(-1)^{\alpha+b}3^b(2l-2\alpha)!}{2^{b-1}\alpha!(l-\alpha)!(l-b-2\alpha)!}\sum_i \frac{(-1)^i(i+3\alpha)!}{i!(b-i)!(i+3\alpha-l-1)!}$$
$$= \frac{(-1)^{\alpha}3^b(2l-2\alpha)!(3\alpha)!}{2^{b-1}\alpha!b!(l+1-b)!(l-\alpha)!(b+3\alpha-l-1)!(l-b-2\alpha)!}.$$

Because of the factorials in the denominator, these coefficients vanish except for integer values of α which satisfy the inequalities

$$2\alpha \leqslant (l-b) \leqslant 3\alpha - 1$$

and it is seen that this excludes $\alpha = 0$ and also $b = l$ and $l - 1$ so that no term of higher power than x^{l-2} can occur. But the vector space defined by these limits is spanned by the solutions for smaller l-values $(l - 2)$, $(l - 4), \ldots$. Hence the solution obtained above, by the $(l + 1)$th application of Q_-, is simply a linear combination of solutions for smaller l.

Appendix B. The proof of a conjecture

What follows is an outline of the proof that (44) is a solution of (43). Consider first the terms on the right-hand side of (43) which involve $B_{i+1}(n, b', r')$. After substitution of (44) these may be collected over a common denominator $t!(n-b-i-2r-2t)!(b+2r+t)!(t+r-i-1)!$ which is just that appropriate to $B_{i+1}(n+1, b, r)$. This process is facilitated by making the transformation $t \to t - 1$ in the two terms having $b' + 2r' = b + 2r + 1$, in this way absorbing the factor $-1/12$ into the summation. The sum of these five terms is then found to be

$$\{1 - 3(i+1)/(n+1)\}(b+2r)B_{i+1}(n+1, b, r).$$

Table 2. The coefficients (46) in the Legendre expansion of the solutions.

I	n_-	$b\,r = 0\,0$	$0\,1$	$0\,2$	$1\,0$
0	0	1	–	–	–
2	0	$-3(l+1)$	–	–	3
4	0	$15(l+1)(l+2)/2$	$-3/2$	–	$-18(l+2)$
	1	$-21l(l+1)/2$	$-3/2$	–	-21
6	0	$-3(l+1)(l+2)(9l+35)/2$	$3(9l+19)/2$	–	$297(l+2)(l+3)/4$
	1	$63l(l+1)(l+2)/2$	$9(l+4)/2$	–	$-9(l+2)(15l-43)/4$
8	0	$9(l+1)(l+2)(l+3)(3l+140)/8$	$-9(l+3)(17l+36)/2$	$9/8$	$-9(l+2)(l+3)(27l+116)$
	1	$-9l(l+1)(l+2)(69l+239)/8$	$9(l^2-22l-51)/2$	$9/8$	$9(l+2)(l+3)(90l-167)/4$
	2	$891(l-1)l(l+1)(l+2)/8$	$9\{7l(l+1)-31\}/2$	$9/8$	$1287\{l(l+1)-2\}/2$

I	n_-	$b\,r = 1\,1$	$2\,0$	$2\,1$	$3\,0$	$4\,0$
0	0	–	–	–	–	–
2	0	–	–	–	–	–
4	0	–	9	–	–	–
	1	–	9	–	–	–
6	0	$-27/4$	$-81(l+3)$	–	27	–
	1	$-27/4$	$-9(3l+20)$	–	27	–
8	0	$9(9l+28)$	$459(l+3)(l+4)$	-27	$-324(l+4)$	81
	1	$9(18l+85)/4$	$-27(l+3)(l-41)$	-27	$-81(2l+13)$	81
	2	$315/2$	$9\{-21l(l+1)+269\}$	-27	-918	81

The sum of the remaining terms, involving the $B_i\left(n, b', r'\right)$, can be separated into a part proportional to $b + 2r$ and one proportional to $2r$. The latter proves to be proportional to $b + 2r$ also and the sum of all these terms is found, after some algebra, to be

$$3(i+1)(b+2r)B_{i+1}(n+1, b, r)/(n+1).$$

Together with the previous result, this verifies that (44) is a solution of (43).

Appendix C. The solutions for even $I \leqslant 8$

Although formula (46) for the coefficients $a_l\,(n, b, r)$ in the general solution involves several summations, the sums are quite simple for small I and the results are listed in table 2 for $I \leqslant 8$. They are given as functions of l for each I and $n_- = 1/2\;(3l - \lambda) + I/4$, which fixes λ. The table is restricted to $n_- \leqslant I/4$ since, as explained in section 4.2, results for $n'_- = I/2 - n_-$ are obtained from those for n_- by the replacement of l by $-(l+1)$. Note that the coefficients for the cases $n_- = I/4$ depend on l only through $l(l+1)$ which is invariant under this reflection.

Appendix D. The norms and overlaps for $I \leqslant 8$

In section 4.3 we described the direct method for calculating the norms of solutions (45) although for small I there are various short cuts. For reference we give the norms and overlaps in tables 3 and 4. As explained before, we use the volume element $\mathrm{d}V = \sin 3\gamma\,\mathrm{d}\gamma\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi\,\mathrm{d}\psi$ and the tables give the values of the norms and overlaps multiplied by $(2I+1)/8\pi^2$. It is

Table 3. Some norms.

I	n_-	$\langle n_- lI \mid n_- lI \rangle\,(2I+1)/8\pi^2$
0	0	$2/3(2l+1)$
2	0	$6(l+1)$
4	0	$54(l+1)(l+2)(6l+5)/7$
	1	$9l(l+1)(6l+1)(6l+5)/5(2l+1)$
6	0	$6(l+1)(l+2)(6l+5)(6l+7)(1098l^2+4941l+5005)/385(2l+3)$
	1	$54l(l+1)(l+2)(6l+1)(6l+7)/11$
8	0	$54(l+1)(l+2)(l+3)(6l+5)(6l+7)(4986l^2+27423l+30940)/5005$
	1	$27l(l+1)(l+2)(6l+1)(6l+5)(9846l^2+44307l+45331)/10010$
	2	$81(l-1)l(l+1)(l+2)(6l-1)(6l+1)(6l+5)(6l+7)/65(2l+1)$

Table 4. Some overlaps.

I	n_-	$\langle n_-+3\; l+2\; I \mid n_- lI \rangle\,(2I+1)/8\pi^2$
6	0	$48(l+1)(l+2)(6l+5)(6l+7)(6l+11)(6l+13)/385(2l+3)$
8	0	$1728(l+1)(l+2)(l+3)(6l+5)(6l+7)(6l+13)(6l+17)/5005$

Table 5. The allowed Octahedral representations for each I, excluding those with dimension 3.

I	0	2	4	6	8	10	12
Octahedral representation	A_1	E	A_1+E	A_1+A_2+E	A_1+2E	A_1+A_2+2E	$2A_1+A_2+2E$

convenient to use the label n_-, see section 2.3, rather than λ, with $\lambda = 3l + I/2 - 2n_-$. The results are valid for both forms (27) and (46) of the solutions.

Norms for the higher values of n_-, given by replacing the value in the table by $(I/2 - n_-)$, are obtained from those in the table by the substitution $l \to -(l+1)$, see section 4.2, with an overall change of sign. The overlap for $I = 8$, $n_- = 1$ is obtained from that in the table by the substitution $l \to -(l+3)$ with an overall sign change while the $I = 6$ entry is invariant under this operation.

Appendix E. The orthonormal Octahedral basis

From the known character tables for the Octahedral group, the reduction of the $(2I+1)$-dimensional representation of the rotation group into irreducible representations of the Octahedral group is given in table 5 for $I \leqslant 12$.

The three-dimensional Octahedral representations are omitted from this table since it is impossible to construct an overall invariant from them with the remaining variable γ. The total dimension in the table, for each I, is $(1/2I+1)$ which is equal to the number of non-negative values of K. Generally, the number of times that each representation occurs is given by $n(E) = [(I+4)/6]$, where $[x]$ again denotes the integer part of x, together with the known total

Table 6. The coefficients for the expansion of each Octahedral representation into Φ_{IIK}.

		A_1 and E_1			A_2 and E_2	
I	Representation	$K=0$	4	8	2	6
0	A	1	–	–	–	–
2	E	1	–	–	1	–
4	A	$(\sqrt{7}$	$\sqrt{5})/2\sqrt{3}$	–	–	–
	E	$(\sqrt{5}$	$-\sqrt{7})/2\sqrt{3}$	–	-1	–
6	A	(1	$-\sqrt{7})/2\sqrt{2}$	–	$(\sqrt{11}$	$-\sqrt{5})/4$
	E	$(\sqrt{7}$	$1)/2\sqrt{2}$	–	$(\sqrt{5}$	$\sqrt{11})/4$
8	A	$(3\sqrt{11}$	$2\sqrt{7}$	$\sqrt{65})/8\sqrt{3}$	–	–
	E	$(-3\sqrt{35}$	$-2\sqrt{55}$	$\sqrt{1001})/16\sqrt{6}$	1	–
	E'	$(-\sqrt{143}$	$2\sqrt{91}$	$\sqrt{5})/16\sqrt{2}$	–	1

Table 7. The expansion of the vectors $|y^{\pm}\rangle$ in the orthonormal Octahedral basis of table 6.

I	y	A_1	A_2	E_1	E_2	E_1'	E_2'
2	0^+	–	–	$\sqrt{2}$	–	–	–
	0^-	–	–	–	$\sqrt{2}$	–	–
4	0^+	–	–	$\sqrt{(6/7)}$	–	–	–
	1^+	$\sqrt{(3/10)}$	–	–	–	–	–
	0^-	–	–	–	$-\sqrt{(6/7)}$	–	–
6	0^+	$3\sqrt{(2/77)}$	–	–	–	–	–
	1^+	–	–	$\sqrt{(2/11)}$	–	–	–
	0^-	–	$\sqrt{(2/5)}$	–	–	–	–
	1^-	–	–	–	$\sqrt{(2/11)}$	–	–
8	0^+	–	–	$9\sqrt{3}/2\sqrt{1001}$	–	$-1/2\sqrt{5}$	–
	1^+	–	–	$-15\sqrt{3}/4\sqrt{1001}$	–	$-1/4\sqrt{5}$	–
	2^+	$\sqrt{(3/130)}$	–	–	–	–	–
	0^-	–	–	–	$9\sqrt{3}/2\sqrt{1001}$	–	$-1/2\sqrt{5}$
	1^-	–	–	–	$15\sqrt{3}/4\sqrt{1001}$	–	$1/4\sqrt{5}$

dimension and $n(A_1) - n(A_2) = (1 + (-1)^{I/2})/2$. It is convenient to express these Octahedral functions in terms of the more familiar D-functions

$$|\alpha RIM\rangle = \sqrt{\frac{2I+1}{8\pi^2}} \sum_{K\geqslant 0} c_K^{\alpha RI}\, \Phi_{IMK}$$

where the Φ_{IMK} where defined in equation (2). With the help of the Octahedral group operators, we find the coefficients given in table 6.

Since A_1 and the first component E_1 of the E representation contain only $K = 0, 4, 8$, etc while A_2 and the second component E_2 contain only $K = 2, 6$, etc their coefficients are given on the left- and right-hand sides of the table respectively. The two E-representations for $I = 8$ have been distinguished, arbitrarily, by putting a zero for the $K = 6$ component in E and making E' orthogonal to E. To express our solutions (45) in this Octahedral basis we need to use expansion (58) of the basis $|b\rangle$. For $I \leqslant 8$, this involves only small values of $y \leqslant 2$ and, for such values, the coefficients $G(n, b, y)$ in (58) are simple, $G(n, b, 0) = 1$, $G(n, b, 1) = (n - 2b)$, $G(n, b, 2) = 1/2\{(n - 2b)^2 - n\}$. The expression of the $|y^{\pm}\rangle$, defined just after equation (58), in terms of the orthonormalized Octahedral basis of table 6 is given in table 7.

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