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Three-body angular basis and sum rules for the associated Legendre polynomials

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Abstract. The three-body angular basis has been used to produce two infinite series of identities for the associated Legendre polynomials which are mostly known as two-body objects. The coefficients that are involved in the new sum rules are given in terms of the Clebsh–Gordan coefficients.

1. Introduction

From the so-called 'addition theorem' for the Legendre polynomials (Landau and Lifshitz 1965) we easily find the identity

$$[P_l^0(\cos\theta)]^2 + 2\sum_{m=1}^{l}[P_l^m(\cos\theta)]^2 = (2l+1)/2 \tag{1}$$

where $P_l^m(\cos\theta)$ are the normalized associated Legendre polynomials. Another identity of a similar nature can be found elsewhere (Varshalovich *et al* 1988)

$$\sum_{m=1}^{l}[mP_l^m(\cos\theta)]^2 = \frac{l(l+1)(2l+1)}{8}\sin^2\theta. \tag{2}$$

The right-hand side of (1) can be thought to be proportional to $[P_0^0(\cos\theta)]^2$ and that of (2) is obviously proportional to $[P_1^1(\cos\theta)]^2$. On the other hand, the left-hand side of both equations looks like the norm of the vector-column, whose components are proportional to $P_l^m(\cos\theta)$.

In the following we introduce three-body hyperspherical harmonics (HH) which, if written in the body-fixed frame, can be factorized into the extrinsic part, depending on three Euler-rotation angles, and the intrinsic one that depends on two hyperangles and describes the deformation of the particle triangle. The optimized form of the intrinsic harmonics (IHH) is a vector-column with components proportional to $P_l^m(\cos\theta)$ where l is the Jacobi-vector angular momentum and m serves as the projection of the total three-body angular momentum J onto the body-fixed z-axis. The total parity quantum number p also influences the vector-column dimension. The scalar product of two vector-columns corresponding to a given (J, p)-pair should not depend on the choice of the quantization axis. This fact allows one to produce two infinite series of the declared sum rules. In two simplest cases: one for normal parity states ($p = (-)^J$) and the other for abnormal parity states ($p = -(-)^J$) we find (1) and (2), respectively. It is worth noting that the derivation is strongly related to a formal quantum description of a free three-body problem in hyperspherical coordinates.

2. Three-body hyperspherical harmonics

For a three-body system $a + b + c$ we introduce a Jacobi vector-pair $\boldsymbol{X}$ and $\boldsymbol{x}$, where $\boldsymbol{X}$ is the position vector of particle b relative to a and $\boldsymbol{x}$ is the position vector of particle c relative to the centre of mass of $a + b$. Then, the hyperradius R and the corresponding reduced masses M and μ are given by

$$MR^2 = MX^2 + \mu x^2 \tag{3}$$

$$\frac{1}{M} = \frac{1}{m_a} + \frac{1}{m_b} \qquad \frac{1}{\mu} = \frac{1}{m_c} + \frac{1}{m_a + m_b}. \tag{4}$$

The mass factor in the left-hand side of the definition (3) is generally the free parameter of the method. Its particular choice does not influence the discussion below. The kinetic energy operator in the centre-of-mass system then reads

$$T = -\frac{1}{2M}\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + \frac{\Lambda^2}{2MR^2}. \tag{5}$$

The most commonly used space-fixed total set of five hyperangles is $\{\alpha, \hat{\boldsymbol{x}}, \hat{\boldsymbol{X}}\}$, where $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{X}}$ define the polar angles of the corresponding vector direction and

$$\alpha = \arctan\left(\frac{\sqrt{M}X}{\sqrt{\mu}x}\right). \tag{6}$$

In this case

$$\Lambda^2 = -\frac{1}{\sin^2 2\alpha}\frac{\partial}{\partial\alpha}\sin^2 2\alpha\frac{\partial}{\partial\alpha} + \frac{\boldsymbol{l}^2}{\cos^2\alpha} + \frac{\boldsymbol{L}^2}{\sin^2\alpha} \tag{7}$$

where $\boldsymbol{l} = -\mathrm{i}\boldsymbol{x} \times \nabla_x$, $\boldsymbol{L} = -\mathrm{i}\boldsymbol{X} \times \nabla_X$ are the corresponding angular momenta, and the volume element is given by the expression

$$\mathrm{d}v = R^5\,\mathrm{d}R\,\mathrm{d}\hat{o} \qquad \mathrm{d}\hat{o} = (\sin\alpha\cos\alpha)^2\mathrm{d}\alpha\,\mathrm{d}\hat{\boldsymbol{x}}\,\mathrm{d}\hat{\boldsymbol{X}}. \tag{8}$$

The HH are defined as solutions of the hyperangular part of the free Schrödinger equation

$$[\Lambda^2 - K(K+4)]\boldsymbol{Y}_K(\hat{o}) = 0 \qquad K = 0, 1, \ldots \tag{9}$$

with the quantum number of the grand angular momentum K. For the chosen set of variables we have the well known analytic form of the non-normalized HH

$$\boldsymbol{Y}_{KlL}^{JpM_J}(\alpha, \hat{\boldsymbol{x}}, \hat{\boldsymbol{X}}) = f_{KlL}(\alpha)\mathcal{Y}_{lL}^{JpM_J}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{X}}) \tag{10}$$

with bipolar harmonics defined by

$$\mathcal{Y}_{lL}^{JpM_J}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{X}}) = [1 + p(-)^{l+L}]\sum_{m,m'} Y_{lm}(\hat{\boldsymbol{x}})Y_{Lm'}(\hat{\boldsymbol{X}})(l, L, m, m'|J, M_J) \tag{11}$$

and

$$f_{KlL}(\alpha) = \cos^l\alpha\sin^L\alpha\, F\left(-n, \frac{K+l+L+4}{2}, L + \frac{3}{2}; \sin^2\alpha\right). \tag{12}$$

Here, the first parameter of the hypergeometric function F, $n = (K - L - l)/2$, should be non-negative.

3. Optimized angular basis set

As Schwartz (1961) demonstrated, only a small set of values $\{l, L\}$ is meaningful in (11) if the ansatz (10) is to be used as the angular part of the three-body wave-function. The corresponding values should satisfy

$$L + l = J \qquad \text{if } p = (-)^J \qquad \text{(normal parity case)} \tag{13}$$

or

$$L + l = J + 1 \qquad \text{if } p = -(-)^J \qquad \text{(abnormal parity case).} \tag{14}$$

As follows from (10) (Matveenko and Fukuda 1998), in the hyperspherical approach this constraint is equivalent to the condition, see (12),

$$n = 0 \tag{15}$$

the condition that suppresses the α-motion.

We also note that HH (11) are formally simpler in the rotated frame when the body-fixed z-axis coincides with one of the Jacobi vectors: $\boldsymbol{X}$ or $\boldsymbol{x}$. Thus, for example, if we choose $\boldsymbol{X}$ as a z-axis we find

$$\boldsymbol{Y}_{KlL}^{JpM_J}(\alpha, \cos\theta, \gamma, \beta, \tilde{\alpha}) = \sum_{m'=0(1)}^{J} y_{KlLm'}^{Jp}(\alpha, \cos\theta) B_{m'}^{JpM_J}(\gamma, \beta, \tilde{\alpha}) \tag{16}$$

where $\{\tilde{\alpha}, \beta, \gamma\}$ defines the corresponding space- to body-fixed rotation, and $B_{m'}^{JpM_J}$ is the parity-preserving combination of the Wigner D-functions (Matveenko and Fukuda 1996).

After substituting this form into the eigenvalue equation (9) and integrating over the Euler angles, we arrive at the system of Schrodinger equations for the IHH, i.e. vector column $||y(\alpha, \cos\theta)||$. Here, we use the analytic form of the solution (Matveenko and Fukuda 1996) and note that owing to (13) or (14) we need only one index l to number the states of a given (J, p)-symmetry

$$||y||_l^{Jp} = (\sin\alpha)^l (\cos\alpha)^L \begin{pmatrix} U_{0L}^{Jpl} \; P_l^0(\cos\theta) \\ U_{1L}^{Jpl} \; P_l^1(\cos\theta) \\ \cdots \\ U_{lL}^{Jpl} \; P_l^l(\cos\theta) \\ 0 \\ \cdots \\ 0 \end{pmatrix} \tag{17}$$

where the coefficients

$$U_{mL}^{Jpl} = p(-)^{J+l+m}\sqrt{2 - \delta_{0m}}(l, J, -m, m|L, 0) \qquad \left(\sum_{m=0}^{l} (U_{mL}^{Jpl})^2 = 1\right) \tag{18}$$

were defined by Chang and Fano (1972) and $\cos\theta = (\boldsymbol{X}\boldsymbol{x})/(Xx)$.

4. Sum rules

The solutions in the form (17) having the same (J, p)-symmetry are, of course, orthogonal and can be normalized. The scalar product should include the summation over the projection m of the total angular momentum onto the body-fixed z-axis and further integration over the (α, θ)-variables. The sum over m is formally equivalent to the matrix multiplication of the vector-column IHH (17) and the corresponding conjugate IHH. This operation produces a scalar function of two variables which no longer depends on the choice of the quantization axis.

As we are not also interested in the α-dependence, therefore we form the partial scalar product by summing over m and integrating over α to obtain a 'bilinear' form

$$\sigma^{Jp}_{l_1 l_2}(\theta) = \sum_{m}^{\min(l_1,l_2)} U^{Jpl_1}_{mL_1} \; P^m_{l_1}(\cos\theta) U^{Jpl_2}_{mL_2} P^m_{l_2}(\cos\theta) \tag{19}$$

here L_1 and L_2 are given by (13) or (14) depending on parity. The key point is that we can produce this form twice for a given pair of IHH: (a) first keeping the Jacobi vector $\boldsymbol{X}$ as the quantization axis and (b) using $\boldsymbol{x}$ for that purpose. We should also take care to ensure that when changing the quantization axis we also interchange the position of l and L quantum numbers in (17).

The final result is split into two series of sum rules for the associated Legendre polynomials. In accordance with (13), for states of the normal parity ($p = n$) we have

$$\sigma^{Jn}_{l_1 l_2}(\theta) = \sigma^{Jn}_{J-l_1, J-l_2}(\theta) \qquad J = 0, 1 \ldots \tag{20}$$

where the summation in (19) starts with $m = 0$. For $p = a$ (abnormal parity states) the lowest possible value of the magnetic quantum number $m = 1$ and the sum rules read, see (14),

$$\sigma^{Ja}_{l_1 l_2}(\theta) = \sigma^{Ja}_{J+1-l_1, J+1-l_2}(\theta) \qquad J = 1, 2 \ldots. \tag{21}$$

The underlying expression (19) forms a symmetrix matrix which has the dimension $(J + 1, J + 1)$ for normal parity states and (J, J) for those of the abnormal parity. Thus, equations (20) and (21) can be considered as relations between the corresponding matrix elements. The total number of equalities is evidently proportional to J^2. The majority of them should be new. In section 5, we consider only simple examples when at least one of the indices is the smallest.

5. Discussion and conclusion

Both results: the normal parity case (20) and the abnormal parity one (21) were checked numerically. Chang and Fano's (1972) coefficients, which are involved in the calculation, are not complicated. If $p = (-)^J$ (normal parity), $L = J - 1$ and

$$U^{Jnl}_{mL} = \left(\frac{2}{1+\delta_{m0}} \frac{(2l)!(2L+1)!(J-m)!(J+m)!}{(2J+1)!(l-m)!(l+m)!(L!)^2} \right)^{1/2} \tag{22}$$

otherwise, if $p = -(-)^J$, we have $L = J - l + 1$ and

$$U^{Jal}_{mL} = 2Lm \left(2(2L+1) \frac{(2l-1)!(2L-1)!(J-m)!(J+m)!}{(2J+2)!(l-m)!(l+m)!(L!)^2} \right)^{1/2}. \tag{23}$$

If $l_1 = l_2 = 0$, our sum rules (20) become simpler. Thus, using (22) we have

$$U^{Jn0}_{0J} = 1 \qquad \text{and} \qquad U^{JnJ}_{m0} = \left(\frac{2}{(1+\delta_{m0})(2J+1)} \right)^{1/2} \tag{24}$$

so that $\sigma(\theta)^{Jn}_{00} = \sigma(\theta)^{Jn}_{JJ}$ is equivalent to (1). Similarly, using (23) for the abnormal parity case (now $l_1 = l_2 = 1$ is the simplest case) we derive

$$U^{Ja1}_{1J} = 1 \qquad \text{and} \qquad U^{JaJ}_{m1} = m \left(\frac{6}{J(J+1)(2J+1)} \right)^{1/2} \tag{25}$$

and $\sigma(\theta)^{Ja}_{11} = \sigma(\theta)^{Ja}_{JJ}$ provides (2).

We conclude the paper by exposing several simple non-diagonal formulae, all having one index in (20) or (21) to be the smallest. For normal parity states we obtain from $\sigma(\theta)^{Jn}_{0l} = \sigma(\theta)^{Jn}_{J,J-l}$ the peculiar form for $P^0_l(\cos\theta)$

$$P^0_l(\cos\theta) = \frac{\sqrt{2}}{\sqrt{2J+1}} \sum_{m=0}^{J-l} \sqrt{\frac{2}{1+\delta_{m0}}} \frac{U^{Jn,J-l}_{ml}}{U^{Jnl}_{0,J-l}} P^m_J(\cos\theta) P^m_{J-l}(\cos\theta). \tag{26}$$

Similarly for abnormal parity states we obtain from $\sigma(\theta)^{Ja}_{1l} = \sigma(\theta)^{Ja}_{J,J-l+1}$

$$U^{Ja1}_{1J} U^{Jal}_{1,J-l+1} P^1_l(\cos\theta) P^1_1(\cos\theta) = \sum_{m=1}^{J-l+1} U^{JaJ}_{m1} U^{Ja,J-l+1}_{ml} P^m_J(\cos\theta) P^m_{J-l+1}(\cos\theta) \tag{27}$$

with U^{JaJ}_{m1} given by (25).

If we take $l = J-1$, we have from (26)

$$P^0_{J-1}(\cos\theta) = \left[\sqrt{2J-1}\cos\theta P^0_J(\cos\theta) - \sqrt{\frac{J+1}{J}}\sin\theta P^1_J(\cos\theta)\right] / \sqrt{2J+1} \tag{28}$$

and from (27)

$$P^1_{J-1}(\cos\theta) = \sqrt{\frac{2J-1}{(J+1)(2J+1)}} [\sqrt{J-1}\cos\theta P^1_J(\cos\theta) - \sqrt{J+2}\sin\theta P^2_J(\cos\theta)]. \tag{29}$$

These two equations look like and are recurrence relations.

The latter two simple formulae are derived as follows. First by putting $l = 2$ into (26) and, making the substitution $J = l-1$ in the final result, in order to compare with Varshalovich *et al* (1988), we arrive at

$$\frac{l(l+1)}{2\sqrt{10}} P^0_2(\cos\theta) = \sum_{m=0}^{l-1} \frac{1}{1+\delta_{m0}} \sqrt{\frac{(l^2-m^2)[(l+1)^2-m^2]}{(2l-1)(2l+3)}} P^m_{l+1}(\cos\theta) P^m_{l-1}(\cos\theta). \tag{30}$$

Second by putting $l = 3$ in (27) for the abnormal counterpart of (30) we find

$$\frac{(J-2)(J-1)J(J+1)}{6\sqrt{14}} P^1_1(\cos\theta) P^1_3(\cos\theta) = \sum_{m=1}^{J-2} m^2 \sqrt{\frac{(J^2-m^2)[(J-1)^2-m^2]}{(2J-3)(2J+1)}} P^m_J(\cos\theta) P^m_{J-2}(\cos\theta). \tag{31}$$

In conclusion, we note that the special three-body angular basis can be given in the form including the associated Legendre polynomials. The partially fulfilled scalar product for states from the basis can be used to produce new sum rules including the normalized $P^m_l(\cos\theta)$ and the Clebsh–Gordan coefficients (Varshalovich *et al* 1988). All the formulae presented, except for (1), (2) and (30) and several trivial cases of (20) and (21), are thought to be new.

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