Rotational invariants constructed by the products of three spherical harmonic polynomials*

MA Zhong-Qi(马中骐)[1,2;1)] YAN Zong-Chao(严宗朝)[3,4;2)]

[1] Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China
[2] Institute for Advanced Study, Tsinghua University, Beijing 100084, China
[3] Department of Physics, University of New Brunswick, Fredericton, New Brunswick, E3B 5A3, Canada
[4] Center for Cold Atom Physics, Chinese Academy of Sciences, Wuhan 430071, China

Abstract: The rotational invariants constructed by the products of three spherical harmonic polynomials are expressed generally as homogeneous polynomials with respect to the three coordinate vectors in the compact form, where the coefficients are calculated explicitly in this paper.

Key words: the rotational invariant, the spherical harmonic polynomial, the homogeneous polynomial

PACS: 02.30.Gp, 03.65.Fd, 02.20.Qs **DOI:** 10.1088/1674-1137/39/6/063104

1 Introduction

Weyl (see p.53 of Ref. [1]) established a theorem on the important structure for rotational invariants: Every even invariant depending on n vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\cdots$, $\boldsymbol{r}_n$ in the three-dimensional space $\mathcal{R}_3$ is expressible in terms of the n^2 scalar products $\boldsymbol{r}_a\cdot\boldsymbol{r}_b$. Every odd invariant is a sum of terms

$$[(\boldsymbol{r}_a\times\boldsymbol{r}_b)\cdot\boldsymbol{r}_c]I(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_n), \tag{1}$$

where $\boldsymbol{r}_a$, $\boldsymbol{r}_b$, $\boldsymbol{r}_c$ are selected from $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\cdots$, $\boldsymbol{r}_n$, and $I(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_n)$ is an even invariant. Due to the property of the rotational group $SO(3)$, the expression for the invariant $I(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_n)$ is not unique except for $n\leqslant 3$ because it depends upon the coupling orders of n vectors $\boldsymbol{r}_a$. In their famous Encyclopedia of Mathematics Vol. 9 on the Racah-Wigner algebra in quantum theory [2], Biedenharn and Louck studied the most important case $n=3$ of the general theorem in some detail (§6.17 of Ref. [2]), and defined the even invariant (see (6.153) of Ref. [2]) as

$$\begin{aligned} &I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)\\ &=\sqrt{\frac{(4\pi)^3}{(2j+1)(2k+1)(2\ell+1)}}\\ &\quad\times\sum_{\mu,\nu,\rho}\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}\mathcal{Y}^j_\mu(\boldsymbol{r}_1)\mathcal{Y}^k_\nu(\boldsymbol{r}_2)\mathcal{Y}^\ell_\rho(\boldsymbol{r}_3)\\ &=\sum_{(\alpha)}A_{(\alpha)}\prod_{a\leqslant b}(\boldsymbol{r}_a\cdot\boldsymbol{r}_b)^{\alpha_{ab}}, \end{aligned} \tag{2}$$

where $\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}$ is the Wigner 3-j symbol, ρ has to be equal to $-\mu-\nu$ owing to the property of the 3-j symbol, $\mathcal{Y}^j_\mu(\boldsymbol{r})$ denotes the spherical harmonic polynomial, and $\sum\alpha_{ab}=(j+k+\ell)/2$. The odd invariant $I_{j,k,\ell}$ is proportional to an even invariant multiplied by a factor $(\boldsymbol{r}_1\times\boldsymbol{r}_2)\cdot\boldsymbol{r}_3$. However, Biedenharn and Louck pointed out in their book (p.308 of [2]) that: "Unfortunately, the expression for the general coefficients (6.157) has not been given in the literature, and one has had to work out these invariant polynomials from the definition, Eq. (6.153)", where the coefficients (6.157) mean $A_{(\alpha)}$.

From the definition, the calculation for $I_{j,k,\ell}$ can be simplified by a special rotation where $\boldsymbol{r}_1$ points to the z-axis and $\boldsymbol{r}_2$ is in the xz plane with non-negative x-component, so that the invariant $I_{j,k,\ell}$ is expressed as a product of two special functions (see Appendix A). In 1987 Fromm and Hill [3] pointed out this method from the definition. In 2004, Harris [4] calculated the even invariants $I_{j,k,\ell}$ with the result containing a coefficient C_j to be determined (see (20) in Ref. [4]), and left the odd invariants $I_{j,k,\ell}$ uncalculated.

The purpose of this paper is to present an independent calculation of the coefficients $A_{(\alpha)}$ in (2) for both even and odd rotational invariants $I_{j,k,\ell}$ generally in a compact form in terms of the internal variables using group theoretical method. Before calculation, we will sketch the reason why $I_{j,k,\ell}$ have widespread applications in many branches of physics, such as in atomic

Received 9 September 2014, Revised 28 November 2014
* Supported by National Natural Science Foundation of China (11174099, 11075014) and NSERC of Canada
1) E-mail: mazq@ihep.ac.cn
2) E-mail: zyan@unb.ca

physics [3, 5–7], in nuclear reaction [2], in condensed matter physics [8], in cosmology [9], and in astronomy and astrophysics [10–12].

After separating the center of mass motion there are three Jacobi coordinate vectors $\boldsymbol{r}_j$ in a four-body system. The independent internal variables are denoted by [13]

$$\eta_1=\boldsymbol{r}_2\cdot\boldsymbol{r}_3,\quad \eta_2=\boldsymbol{r}_3\cdot\boldsymbol{r}_1,\quad \eta_3=\boldsymbol{r}_1\cdot\boldsymbol{r}_2,$$

$$\xi_1=\boldsymbol{r}_1\cdot\boldsymbol{r}_1,\quad \xi_2=\boldsymbol{r}_2\cdot\boldsymbol{r}_2,\quad \zeta=(\boldsymbol{r}_1\times\boldsymbol{r}_2)\cdot\boldsymbol{r}_3, \tag{3}$$

where ζ has odd parity and the remaining have even parity. Due to the identity [13]

$$\zeta^2=\xi_1\xi_2\xi_3-\xi_1\eta_1^2-\xi_2\eta_2^2-\xi_3\eta_3^2+2\eta_1\eta_2\eta_3, \tag{4}$$

with $\xi_3=\boldsymbol{r}_3\cdot\boldsymbol{r}_3$, the invariant ζ may be replaced by ξ_3 in (2) for the even invariant $I_{j,k,\ell}(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3)$. Thus, a measurable physical quantity in a four-body system is generally proportional to

$$T^{jk\ell}_{\mu\nu\rho}=\int(\mathrm{d}\xi)(\mathrm{d}\eta)(\mathrm{d}R)G(\xi,\eta)\mathcal{Y}^j_\mu(\boldsymbol{r}_1)\mathcal{Y}^k_\nu(\boldsymbol{r}_2)\mathcal{Y}^\ell_\rho(\boldsymbol{r}_3), \tag{5}$$

where $G(\xi,\eta)$ is a rotational invariant depending on the internal variables, $(\mathrm{d}\xi)(\mathrm{d}\eta)$ is the integral element for the six internal variables, and $(\mathrm{d}R)=\sin\beta\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\gamma/(8\pi^2)$ is the integral element for the Euler angles. From group theory [14], for a spatial rotation R,

$$\begin{aligned}&P_R\left[\mathcal{Y}^j_\mu(\boldsymbol{r}_1)\mathcal{Y}^k_\nu(\boldsymbol{r}_2)\mathcal{Y}^\ell_\rho(\boldsymbol{r}_3)\right]\\ =&\sum_{\mu'\nu'\rho'}\mathcal{Y}^j_{\mu'}(\boldsymbol{r}_1)\mathcal{Y}^k_{\nu'}(\boldsymbol{r}_2)\mathcal{Y}^\ell_{\rho'}(\boldsymbol{r}_3)\\ &\times D^j_{\mu'\mu}(R)D^k_{\nu'\nu}(R)D^\ell_{\rho'\rho}(R),\end{aligned}$$

$$\begin{aligned}&\int(\mathrm{d}R)D^j_{\mu'\mu}(R)D^k_{\nu'\nu}(R)D^\ell_{\rho'\rho}(R)\\ =&\begin{pmatrix} j & k & \ell\\ \mu' & \nu' & \rho'\end{pmatrix}\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}.\end{aligned}$$

Thus, the rotational variables are separated

$$\begin{aligned}T^{jk\ell}_{\mu\nu\rho}=&\sqrt{\frac{(2j+1)(2k+1)(2\ell+1)}{(4\pi)^3}}\\ &\times\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}\int(\mathrm{d}\xi)(\mathrm{d}\eta)G(\xi,\eta)I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3).\end{aligned} \tag{6}$$

It is therefore desirable to re-express $I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ in terms of a polynomial of the internal variables ξ_i and η_i. Finding such a polynomial may not be an easy task, particularly for higher arbitrary values of $\{j,k,\ell\}$.

The plan of this paper is as follows. The general properties of these invariants are listed in Section 2. The coefficients $A_{(\alpha)}$ for even and odd invariants are calculated in Section 3 and Section 4, respectively. The conclusions are given in Section 5. In the Appendix the invariants $I_{j,k,\ell}$ are calculated from their definition and are expressed as the products of two special functions.

2 General properties of the invariants

For any given three non-negative integers j, k, and ℓ, satisfying the "triangle rule":

$$|j-k|\leqslant\ell\leqslant j+k, \tag{7}$$

the rotational invariant $I_{j,k,\ell}(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3)$ constructed from the products of three spherical harmonic polynomials is defined in (2). The invariant $I_{j,k,\ell}(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3)$ has the following properties.

a) $I_{j,k,\ell}(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3)$ is a homogeneous polynomial of orders j, k, and ℓ with respect to the coordinate vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$, respectively.

b) The parity of $I_{j,k,\ell}(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3)$ is $(-1)^{j+k+\ell}$.

c) Due to the symmetry of the Wigner 3-j symbol

$$\begin{aligned}(-1)^{j+k+\ell}\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}=&\begin{pmatrix} k & j & \ell\\ \nu & \mu & \rho\end{pmatrix}=\begin{pmatrix} j & \ell & k\\ \mu & \rho & \nu\end{pmatrix}\\ =&\begin{pmatrix} j & k & \ell\\ -\mu & -\nu & -\rho\end{pmatrix},\end{aligned}$$

we have

$$\begin{aligned}(-1)^{j+k+\ell}I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)=&I_{k,j,\ell}(\boldsymbol{r}_2,\boldsymbol{r}_1,\boldsymbol{r}_3)\\ =&I_{j,\ell,k}(\boldsymbol{r}_1,\boldsymbol{r}_3,\boldsymbol{r}_2).\end{aligned} \tag{8}$$

Thus, we need only consider $I_{j,k,\ell}$ with $j\leqslant k\leqslant\ell$. For the sake of convenience, we write an even invariant as $I_{j,k,j+k-2n}$ and an odd invariant as $I_{j+1,k+1,j+k-2n+1}$ where $0\leqslant 2n\leqslant j\leqslant k$.

d) $I_{j,k,j+k-2n}$ is real and $I_{j+1,k+1,j+k-2n+1}$ is pure imaginary because

$$\begin{aligned}&\left[\sum_{\mu\nu\rho}\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}\mathcal{Y}^j_\mu(\boldsymbol{r}_1)\mathcal{Y}^k_\nu(\boldsymbol{r}_2)\mathcal{Y}^\ell_\rho(\boldsymbol{r}_3)\right]^*\\ =&\sum_{\mu\nu\rho}\begin{pmatrix} j & k & \ell\\ \mu & \nu & \rho\end{pmatrix}\mathcal{Y}^j_{-\mu}(\boldsymbol{r}_1)\mathcal{Y}^k_{-\nu}(\boldsymbol{r}_2)\mathcal{Y}^\ell_{-\rho}(\boldsymbol{r}_3).\end{aligned}$$

e) $I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ satisfies the three Laplace's equations with respect to $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$, respectively,

$$\varDelta_1 I_{j,k,\ell}=\varDelta_2 I_{j,k,\ell}=\varDelta_3 I_{j,k,\ell}=0. \tag{9}$$

f) From group theory on $SO(3)$ [14], the decomposition of the direct product of three irreducible representations of $SO(3)$, $D^j(R)\times D^k(R)\times D^\ell(R)$, where j, k, and ℓ satisfy the triangle rule (7), contains one and only one identity representation $D^0(R)$. Thus, a homogeneous polynomial of orders j, k, and ℓ with respect to the coordinate vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$, respectively, which satisfies the Laplace's Eq. (9), does exist and is unique up to a constant factor.

From the explicit formula for the spherical harmonic polynomial [14], we have

$$\mathcal{Y}^k_{\pm 1}(\boldsymbol{r}) = \mp\sqrt{\frac{k(k+1)(2k+1)}{16\pi}}\left\{(x\pm \mathrm{i}y)z^{k-1}+\cdots\right\},$$

$$\mathcal{Y}^k_0(\boldsymbol{r}) = \sqrt{\frac{(2k+1)}{4\pi}}\left\{z^k+\cdots\right\}, \tag{10}$$

where x, y, and z are the three components of $\boldsymbol{r}$. Among all spherical harmonic polynomials $\mathcal{Y}^k_\nu(\boldsymbol{r})$ with k given, the term z^k appears only in $\mathcal{Y}^k_0(\boldsymbol{r})$ and the terms xz^{k-1} and yz^{k-1} appear only in $\mathcal{Y}^k_{\pm1}(\boldsymbol{r})$. Therefore, $z_1^j z_2^k z_3^{j+k-2n}$ is contained only once in the homogeneous polynomial $I_{j,k,j+k-2n}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$, at $\mathcal{Y}^j_0(\boldsymbol{r}_1)\mathcal{Y}^k_0(\boldsymbol{r}_2)\mathcal{Y}^{j+k-2n}_0(\boldsymbol{r}_3)$, with the coefficient

$$\begin{pmatrix} j & k & j+k-2n \\ 0 & 0 & 0 \end{pmatrix}. \tag{11}$$

Thus the even invariant defined in (2) can be rewritten more explicitly in the form

$$\begin{aligned} & I_{j,k,j+k-2n}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) \\ &= \begin{pmatrix} j & k & j+k-2n \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad\times P^{-1}_{j,k,j+k-2n}\sum_{a=0}^{[j/2]}\sum_{b=0}^{j-2a}\sum_{c=\max\{0,n-a-b\}}^{[(k-b)/2]} A_{abc} \\ &\quad\times \xi_1^a\xi_2^c\xi_3^{a+b+c-n}\eta_1^{k-2c-b}\eta_2^{j-2a-b}\eta_3^b, \end{aligned}$$

$$P_{j,k,j+k-2n} = \sum_a\sum_b\sum_c A_{abc}, \tag{12}$$

where $[m]$ denotes the largest integer equal to or less than the non-negative real number m. Similarly, $x_1y_2z_1^jz_2^kz_3^{j+k-2n}$ is contained only twice in the homogeneous polynomial $I_{j+1,k+1,j+k-2n+1}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$, at $\mathcal{Y}^{j+1}_{\pm1}(\boldsymbol{r}_1)\mathcal{Y}^{k+1}_{\mp1}(\boldsymbol{r}_2)\mathcal{Y}^{j+k-2n+1}_0(\boldsymbol{r}_3)$, with the coefficient

$$\frac{\mathrm{i}}{2}\sqrt{\frac{(j+2)!(k+2)!}{j!k!}}\begin{pmatrix} j+1 & k+1 & j+k-2n+1 \\ 1 & -1 & 0 \end{pmatrix}. \tag{13}$$

Thus the odd invariant defined in (2) can be rewritten more explicitly in the form

$$\begin{aligned} & I_{j+1,k+1,j+k-2n+1}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) \\ &= \frac{\mathrm{i}\zeta}{2}\sqrt{\frac{(j+2)!(k+2)!}{j!k!}} \\ &\quad\times \begin{pmatrix} j+1 & k+1 & j+k-2n+1 \\ 1 & -1 & 0 \end{pmatrix} \\ &\quad\times Q^{-1}_{j,k,j+k-2n}\sum_{a=0}^{[j/2]}\sum_{b=0}^{j-2a}\sum_{c=\max\{0,n-a-b\}}^{[(k-b)/2]} B_{abc} \\ &\quad\times \xi_1^a\xi_2^c\xi_3^{a+b+c-n}\eta_1^{k-2c-b}\eta_2^{j-2a-b}\eta_3^b, \end{aligned}$$

$$Q_{j,k,j+k-2n} = \sum_a\sum_b\sum_c B_{abc}. \tag{14}$$

3 Even invariants

The coefficients A_{abc} in (12) are determined from the conditions (9), leading directly to the following recursive relations:

$$\begin{aligned} & 2a(2j-2a+1)A_{abc} \\ & +(j-2a-b+2)(j-2a-b+1)A_{(a-1)bc} \\ & +(b+2)(b+1)A_{(a-1)(b+2)(c-1)} \\ & +2(b+1)(j-2a-b+1)A_{(a-1)(b+1)c}=0, \end{aligned} \tag{15}$$

$$\begin{aligned} & 2c(2k-2c+1)A_{abc} \\ & +(k-2c-b+2)(k-2c-b+1)A_{ab(c-1)} \\ & +(b+2)(b+1)A_{(a-1)(b+2)(c-1)} \\ & +2(b+1)(k-2c-b+1)A_{a(b+1)(c-1)}=0, \end{aligned} \tag{16}$$

$$\begin{aligned} & 2(a+b+c-n)(2k+2j-2a-2b-2c-2n+1)A_{abc} \\ & +(k-2c-b+2)(k-2c-b+1)A_{ab(c-1)} \\ & +(j-2a-b+2)(j-2a-b+1)A_{(a-1)bc} \\ & +2(k-2c-b+1)(j-2a-b+1)A_{a(b-1)c}=0. \end{aligned} \tag{17}$$

Due to the property f) in Sec. 2, the solutions for A_{abc} exist uniquely up to a common numerical factor, which can be determined for convenience by

$$\begin{aligned} A_{00n} &= \frac{(k-n)!(2j-1)!!}{(k-2n)!(2j-2n-1)!!} \\ &\quad\times\prod_{m=1}^{\lambda}2m(2j+2k-4n-2m+1), \end{aligned} \tag{18}$$

$$\lambda=[(j+k)/2]-n. \tag{19}$$

Because of the normalization factor $P_{j,k,j+k-2n}$, the choice for A_{00n} does not matter to the final result of $I_{j,k,j+k-2n}$. The coefficients A_{abc} can be calculated one by one by mathematical induction from the recursive relations (15–17), where the calculation path is critical. The key point is that at each step of calculation using one of (15–17), only one unknown coefficient is solved from the three remaining known coefficients.

In fact, the mathematical inductions are overlapped in the calculations of $A_{a(n-a+b)c}$ and especially of $A_{(n+a)bc}$. Let us consider $A_{a(n-a+b)c}$ for example. One calculates $A_{a(n-a)c}$ by usual mathematical induction through the calculations of $A_{a(n-a)1}$, $A_{a(n-a)2}$, and $A_{a(n-a)d}$ with $0\leqslant d\leqslant c-1$ by (17). Then, one uses the similar method to calculate $A_{a(n-a+1)c}$, $A_{a(n-a+2)c}$ and so on. The difficulty occurs when one calculates $A_{a(n-a+b)c}$ by (17) where $A_{a(n-a+d)c}$ with $0\leqslant d\leqslant b-1$ are assumed to be known. One finds that there are two coefficients $A_{a(n-a+b)c}$ and $A_{a(n-a+b)(c-1)}$ in (17) to be determined. One has to calculate $A_{a(n-a+b)0}$, $A_{a(n-a+b)1}$, $A_{a(n-a+b)2}$, and $A_{a(n-a+b)d}$ with $0\leqslant d\leqslant c-1$. This indicates that the overlapped mathematical inductions occur in calculating $A_{a(n-a+b)c}$, where $A_{a(n-a+b)c}$ is calculated by (17), under two assumptions that both $A_{a(n-a+d)c}$ with $0\leqslant d\leqslant b-1$ and $A_{a(n-a+b)d}$ with $0\leqslant d\leqslant c-1$ are known.

First, we calculate $A_{0b(n-b)}$ from (16), and $A_{ab(n-a-b)}$ from (15) by mathematical induction:

$$A_{ab(n-a-b)} = G_{a,b}\frac{(j-n)!(k-n)!}{(j-2a-b)!(k-2n+2a+b)!}\times\prod_{m=1}^{\lambda}2m(2j+2k-4n-2m+1), \quad (20)$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant n-a$, and

$$G_{a,b} = \sum_{r=\max\{0,2a+b-n\}}^{a}\frac{(-1)^{a+b+r}n!}{2^{a-r}r!(a-r)!b!}\times\frac{(j-2a-b+r)!(k-2n+2a+b)!}{(n-2a-b+r)!(j-n)!(k-2n+2a+b-r)!}\times\frac{(2j-2a-1)!!(2k-2n+4a+2b-2r-1)!!}{(2j-2n-1)!!(2k-2n-1)!!}. \quad (21)$$

Evidently, $G_{a,b}=0$ if $a<0$, or $b<0$, or $a+b>n$. The function $G_{a,b}$ will play an essential role for later calculations.

Second, we calculate $A_{ab(n-a-b+c)}$ from (17) by mathematical induction:

$$A_{ab(n-a-b+c)} = \sum_{s=0}^{c}\sum_{r=s}^{c}G_{a-c+r,b-s}\times\frac{(-1)^{c}2^{s}(c!)(j-n)!(k-n)!}{(c-r)!(r-s)!s!(j-2a-b)!(k-2n+2a+b-2c)!}\times\prod_{m=c+1}^{\lambda}2m(2j+2k-4n-2m+1), \quad (22)$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant n-a$, and $0\leqslant c\leqslant[(k+b)/2]+a-n$. For the case of $c>b$, terms with $b<s\leqslant c$, which may occur in the sum over s in (22), vanish because $G_{a,b}=0$ if $b<0$. For the case of $c>a$, terms with $c-a>r\geqslant s$, which may occur in the sum over r in (22), vanish because $G_{a,b}=0$ if $a<0$. Thus, the upper bound of summation over s in (22) can be replaced equivalently by $\min\{c,b\}$, and the lower bound of summation over r in (22) becomes $\max\{s,c-a\}$. Similar cases occur in the following formulas.

Third, we calculate $A_{a(n-a+b)c}$ from (17) by mathematical induction:

$$A_{a(n-a+b)c} = \sum_{s=\max\{0,b-a\}}^{\min\{b+c,n-a+b\}}\sum_{r=\max\{s,b+c-a\}}^{\min\{s+c,b+c\}}\times G_{a-b-c+r,n-a+b-s}\frac{(-1)^{b+c}2^{s}(b+c)!}{(r-s)!s!(b+c-r)!}\times\frac{(j-n)!(k-n)!}{(j-n-a-b)!(k-n+a-b-2c)!}\times\prod_{m=b+c+1}^{\lambda}2m(2j+2k-4n-2m+1), \quad (23)$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant j-n-a$, and $0\leqslant c\leqslant[(k-n+a-b)/2]$. For the case of $b+c>a$, terms with $s\leqslant r<b+c-a$, which may occur in the sum over r in (23), vanish because $G_{a,b}=0$ if $a<0$. When $s>b$, terms with $b+c<r\leqslant s+c$ vanish due to the existence of the factor $(b+c-r)!$ at the denominator. For the case of $b>a$, terms with $0\leqslant s<b-a$, which may occur in the sum over s in (23), vanish because $G_{a,b}=0$ if $b>n$. Finally, for the case of $c>n-a$, terms with $n-a+b<s\leqslant b+c$, which may occur in the sum over s in (23), vanish because $G_{a,b}=0$ if $b<0$.

Finally, we calculate $A_{(n+a)bc}$ from (17) by mathematical induction:

$$A_{(n+a)bc} = \sum_{s=\max\{0,b-n\}}^{b}\sum_{r=\max\{s,b+c-n\}}^{s+c}\times G_{n-b-c+r,b-s}\frac{(-1)^{a+b+c}2^{s}(a+b+c)!}{(r-s)!s!(a+b+c-r)!}\times\frac{(j-n)!(k-n)!}{(j-2n-2a-b)!(k-2c-b)!}\times\prod_{m=a+b+c+1}^{\lambda}2m(2j+2k-4n-2m+1), \quad (24)$$

where $0\leqslant a\leqslant[j/2]-n$, $0\leqslant b\leqslant j-2n-2a$, and $0\leqslant c\leqslant[(k-b)/2]$. For the case of $b+c>n$, terms with $s\leqslant r<b+c-n$, which may occur in the sum over r in (24), vanish because $G_{a,b}=0$ if $a<0$. For the case of $b>n$, terms with $0\leqslant s<b-n$, which may occur in the sum over s in (24), vanish because $G_{a,b}=0$ if $b>n$.

For $I_{j,k,j+k}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ (the case $n=0$) we have $G_{0,0}=1$

and

$$A_{abc} = \frac{(-1)^{a+b+c}2^b(a+b+c)!j!k!}{a!b!c!(j-2a-b)!(k-2c-b)!} \times \prod_{m=a+b+c+1}^{\lambda} 2m(2j+2k-2m+1). \qquad (25)$$

For $I_{j,k,j+k-2}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ (the case $n=1$) we have $G_{0,0}=j(2j-1)$, $G_{0,1}=-(2j-1)(2k-1)$, $G_{1,0}=k(2k-1)$, and

$$A_{00(1+c)} = \frac{(-1)^c(k-1)!(2j-1)}{(k-2-2c)!} \times \prod_{m=c+1}^{\lambda} 2m(2j+2k-2m-3),$$

$$A_{0(1+b)c} = [2cj-(b+1)(2k-1)](2j-1) \times \frac{(-1)^{b+c}2^b(b+c)!(j-1)!(k-1)!}{(c)!(b+1)!(j-1-b)!(k-1-b-2c)!} \times \prod_{m=b+c+1}^{\lambda} 2m(2j+2k-2m-3).$$

$$A_{(1+a)bc} = [2cj(2j-1)-b(2j-1)(2k-1) +2(a+1)k(2k-1)] \times \frac{(-1)^{a+b+c}2^{b-1}(a+b+c)!(j-1)!(k-1)!}{(a+1)!b!c!(j-2-2a-b)!(k-2c-b)!} \times \prod_{m=a+b+c+1}^{\lambda} 2m(2j+2k-2m-3).$$

In the following we list some even invariants $I_{j,k,j+k-2n}$ for reference.

$$I_{0,0,0} = 1, \qquad I_{0,1,1}=\frac{-1}{\sqrt{3}}\ \eta_1,$$

$$I_{0,2,2} = \frac{1}{\sqrt{5}}\left\{\frac{1}{2}[3\eta_1^2-\xi_2\xi_3]\right\},$$

$$I_{0,3,3} = \frac{-1}{\sqrt{7}}\left\{\frac{1}{2}[5\eta_1^3-3\xi_2\xi_3\eta_1]\right\},$$

$$I_{0,4,4} = \frac{1}{3}\left\{\frac{1}{8}[35\eta_1^4-30\xi_2\xi_3\eta_1^2+3\xi_2^2\xi_3^2]\right\},$$

$$I_{0,5,5} = \frac{-1}{\sqrt{11}}\left\{\frac{1}{8}[63\eta_1^5-70\xi_2\xi_3\eta_1^3+15\xi_2^2\xi_3^2\eta_1]\right\},$$

$$I_{0,6,6} = \frac{1}{\sqrt{13}}\left\{\frac{1}{16}[231\eta_1^6-315\xi_2\xi_3\eta_1^4 +105\xi_2^2\xi_3^2\eta_1^2-5\xi_2^3\xi_3^3]\right\},$$

$$I_{1,1,2} = \sqrt{\frac{2}{15}}\left\{\frac{1}{2}[3\eta_1\eta_2-\xi_3\eta_3]\right\},$$

$$I_{1,2,3} = -\sqrt{\frac{3}{35}}\left\{\frac{1}{2}[5\eta_1^2\eta_2-\xi_2\xi_3\eta_2-2\xi_3\eta_1\eta_3]\right\},$$

$$I_{1,3,4} = \frac{2}{3}\sqrt{\frac{1}{7}}\left\{\frac{1}{8}[35\eta_1^3\eta_2-15\xi_2\xi_3\eta_1\eta_2-15\xi_3\eta_1^2\eta_3 +3\xi_2\xi_3^2\eta_3]\right\},$$

$$I_{1,4,5} = -\frac{1}{3}\sqrt{\frac{5}{11}}\left\{\frac{1}{8}[63\eta_1^4\eta_2-42\xi_2\xi_3\eta_1^2\eta_2 +3\xi_2^2\xi_3^2\eta_2-28\xi_3\eta_1^3\eta_3+12\xi_2\xi_3^2\eta_1\eta_3]\right\},$$

$$I_{1,5,6} = \sqrt{\frac{6}{143}}\left\{\frac{1}{16}[231\eta_1^5\eta_2-210\xi_2\xi_3\eta_1^3\eta_2+35\xi_2^2\xi_3^2\eta_1\eta_2 -105\xi_3\eta_1^4\eta_3+70\xi_2\xi_3^2\eta_1^2\eta_3-5\xi_2^2\xi_3^3\eta_3]\right\},$$

$$I_{2,2,2} = -\sqrt{\frac{2}{35}}\left\{\frac{1}{2}[-3\xi_2\eta_2^2+9\eta_1\eta_2\eta_3-3\xi_3\eta_3^2 -3\xi_1\eta_1^2+2\xi_1\xi_2\xi_3]\right\},$$

$$I_{2,2,4} = \sqrt{\frac{2}{35}}\left\{\frac{1}{8}[35\eta_1^2\eta_2^2-5\xi_2\xi_3\eta_2^2-20\xi_3\eta_1\eta_2\eta_3 +2\xi_3^2\eta_3^2-5\xi_1\xi_3\eta_1^2+\xi_1\xi_2\xi_3^2]\right\},$$

$$I_{2,3,3} = \frac{2}{\sqrt{105}}\left\{\frac{1}{8}[-30\xi_2\eta_1\eta_2^2+75\eta_1^2\eta_2\eta_3-3\xi_2\xi_3\eta_2\eta_3 -30\xi_3\eta_1\eta_3^2-25\xi_1\eta_1^3+21\xi_1\xi_2\xi_3\eta_1]\right\},$$

$$I_{2,3,5} = -\sqrt{\frac{10}{231}}\left\{\frac{1}{8}[63\eta_1^3\eta_2^2-21\xi_2\xi_3\eta_1\eta_2^2-42\xi_3\eta_1^2\eta_2\eta_3 +6\xi_2\xi_3^2\eta_2\eta_3+6\xi_3^2\eta_1\eta_3^2-7\xi_1\xi_3\eta_1^3+3\xi_1\xi_2\xi_3^2\eta_1]\right\},$$

$$I_{2,4,4} = \frac{-2}{3}\sqrt{\frac{5}{77}}\left\{\frac{1}{8}[-63\xi_2\eta_1^2\eta_2^2+9\xi_2^2\xi_3\eta_2^2+147\eta_1^3\eta_2\eta_3 -27\xi_2\xi_3\eta_1\eta_2\eta_3-63\xi_3\eta_1^2\eta_3^2+9\xi_2\xi_3^2\eta_3^2-49\xi_1\eta_1^4 +51\xi_1\xi_2\xi_3\eta_1^2-6\xi_1\xi_2^2\xi_3^2]\right\},$$

$$
\begin{aligned}
I_{2,4,6} = & \sqrt{\frac{5}{143}}\left\{\frac{1}{16}[231\eta_1^4\eta_2^2-126\xi_2\xi_3\eta_1^2\eta_2^2+7\xi_2^2\xi_3^2\eta_2^2\right.\\
& -168\xi_3\eta_1^3\eta_2\eta_3+56\xi_2\xi_3^2\eta_1\eta_2\eta_3+28\xi_3^2\eta_1^2\eta_3^2\\
& \left.-4\xi_2\xi_3^3\eta_3^2-21\xi_1\xi_3\eta_1^4+14\xi_1\xi_2\xi_3^2\eta_1^2-\xi_1\xi_2^2\xi_3^3]\right\},
\end{aligned}
$$

$$
\begin{aligned}
I_{3,3,4} = & -\sqrt{\frac{2}{77}}\left\{\frac{1}{8}[-70\xi_2\eta_1\eta_2^3+175\eta_1^2\eta_2^2\eta_3+5\xi_2\xi_3\eta_2^2\eta_3\right.\\
& -100\xi_3\eta_1\eta_2\eta_3^2+10\xi_3^2\eta_3^3-70\xi_1\eta_1^3\eta_2\\
& \left.+60\xi_1\xi_2\xi_3\eta_1\eta_2+5\xi_1\xi_3\eta_1^2\eta_3-7\xi_1\xi_2\xi_3^2\eta_3]\right\},
\end{aligned}
$$

$$
\begin{aligned}
I_{3,3,6} = & \frac{10}{\sqrt{3003}}\left\{\frac{1}{16}[231\eta_1^3\eta_2^3-63\xi_2\xi_3\eta_1\eta_2^3-189\xi_3\eta_1^2\eta_2^2\eta_3\right.\\
& +21\xi_2\xi_3^2\eta_2^2\eta_3+42\xi_3^2\eta_1\eta_2\eta_3^2-2\xi_3^3\eta_3^3-63\xi_1\xi_3\eta_1^3\eta_2\\
& \left.+21\xi_1\xi_2\xi_3^2\eta_1\eta_2+21\xi_1\xi_3^2\eta_1^2\eta_3-3\xi_1\xi_2\xi_3^3\eta_3]\right\}.
\end{aligned}
$$

4 Odd invariants

Substituting (14) into Laplace's equations (9), we obtain the recursive relations for the coefficients B_{abc}

$$
\begin{aligned}
& 2a(2j-2a+3)B_{abc}\\
& +(j-2a-b+2)(j-2a-b+1)B_{(a-1)bc}\\
& +(b+2)(b+1)B_{(a-1)(b+2)(c-1)}\\
& +2(b+1)(j-2a-b+1)B_{(a-1)(b+1)c}=0, \qquad (26)
\end{aligned}
$$

$$
\begin{aligned}
& 2c(2k-2c+3)B_{abc}\\
& +(k-2c-b+2)(k-2c-b+1)B_{ab(c-1)}\\
& +(b+2)(b+1)B_{(a-1)(b+2)(c-1)}\\
& +2(b+1)(k-2c-b+1)B_{a(b+1)(c-1)}=0, \qquad (27)
\end{aligned}
$$

$$
\begin{aligned}
& 2(a+b+c-n)(2k+2j-2a-2b-2c-2n+3)B_{abc}\\
& +(k-2c-b+2)(k-2c-b+1)B_{ab(c-1)}\\
& +(j-2a-b+2)(j-2a-b+1)B_{(a-1)bc}\\
& +2(k-2c-b+1)(j-2a-b+1)B_{a(b-1)c}=0. \qquad (28)
\end{aligned}
$$

The only difference between the two sets of equations (15–17) and (26–28) is that "+1" in the first term of each equation of the first set is replaced by "+3" in that of the second set. Thus, through the same procedure we have calculated the coefficients B_{abc} listed below, which are very similar to the coefficients A_{abc}.

$$
\begin{aligned}
B_{00n} = & \frac{(k-n)!(2j+1)!!}{(k-2n)!(2j-2n+1)!!}\\
& \times\prod_{m=1}^{\lambda}2m(2j+2k-4n-2m+3). \qquad (29)
\end{aligned}
$$

$$
\begin{aligned}
B_{ab(n-a-b)} = & F_{a,b}\frac{(j-n)!(k-n)!}{(j-2a-b)!(k-2n+2a+b)!}\\
& \times\prod_{m=1}^{\lambda}2m(2j+2k-4n-2m+3), \qquad (30)
\end{aligned}
$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant n-a$, and

$$
\begin{aligned}
F_{a,b} = & \sum_{r=\max\{0,2a+b-n\}}^{a}\frac{(-1)^{a+b+r}n!}{2^{a-r}r!(a-r)!b!}\\
& \times\frac{(j-2a-b+r)!(k-2n+2a+b)!}{(n-2a-b+r)!(j-n)!(k-2n+2a+b-r)!}\\
& \times\frac{(2j-2a+1)!!(2k-2n+4a+2b-2r+1)!!}{(2j-2n+1)!!(2k-2n+1)!!}. \qquad (31)
\end{aligned}
$$

Evidently, $F_{a,b}=0$ if $a<0$, or $b<0$, or $a+b>n$.

$$
\begin{aligned}
& B_{ab(n-a-b+c)}\\
& =\sum_{s=0}^{\min\{c,b\}}\sum_{r=\max\{s,c-a\}}^{c}F_{a-c+r,b-s}\\
& \times\frac{(-1)^c2^s(c!)(j-n)!(k-n)!}{(c-r)!(r-s)!s!(j-2a-b)!(k-2n+2a+b-2c)!}\\
& \times\prod_{m=c+1}^{\lambda}2m(2j+2k-4n-2m+3), \qquad (32)
\end{aligned}
$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant n-a$, and $0\leqslant c\leqslant[(k+b)/2]+a-n$.

$$
\begin{aligned}
& B_{a(n-a+b)c}\\
& =\sum_{s=\max\{0,b-a\}}^{\min\{b+c,n-a+b\}}\sum_{r=\max\{s,b+c-a\}}^{\min\{s+c,b+c\}}\\
& F_{a-b-c+r,n-a+b-s}\frac{(-1)^{b+c}2^s(b+c)!}{(r-s)!s!(b+c-r)!}\\
& \times\frac{(j-n)!(k-n)!}{(j-n-a-b)!(k-n+a-b-2c)!}\\
& \times\prod_{m=b+c+1}^{\lambda}2m(2j+2k-4n-2m+3), \qquad (33)
\end{aligned}
$$

where $0\leqslant a\leqslant n$, $0\leqslant b\leqslant j-n-a$, and $0\leqslant c\leqslant[(k-n+a-b)/2]$.

$$B_{(n+a)bc} = \sum_{s=\max\{0,b-n\}}^{b}\sum_{r=\max\{s,b+c-n\}}^{s+c} F_{n-b-c+r,b-s}\frac{(-1)^{a+b+c}2^s(a+b+c)!}{(r-s)!s!(a+b+c-r)!} \times\frac{(j-n)!(k-n)!}{(j-2n-2a-b)!(k-2c-b)!} \times\prod_{m=a+b+c+1}^{\lambda}2m(2j+2k-4n-2m+3), \quad (34)$$

where $0\leqslant a\leqslant[j/2]-n$, $0\leqslant b\leqslant j-2n-2a$, and $0\leqslant c\leqslant[(k-b)/2]$.

In the following we list some odd invariants.

$$I_{1,1,1} = \frac{\mathrm{i}\zeta}{\sqrt{6}},$$

$$I_{1,2,2} = -\mathrm{i}\zeta\sqrt{\frac{3}{10}}\;\eta_1,$$

$$I_{1,3,3} = \mathrm{i}\zeta\sqrt{\frac{3}{7}}\left\{\frac{1}{4}[5\eta_1^2-\xi_2\xi_3]\right\},$$

$$I_{1,4,4} = -\mathrm{i}\zeta\frac{\sqrt{5}}{3}\left\{\frac{1}{4}[7\eta_1^3-3\xi_2\xi_3\eta_1]\right\},$$

$$I_{1,5,5} = \mathrm{i}\zeta\sqrt{\frac{15}{22}}\left\{\frac{1}{8}[21\eta_1^4-14\xi_2\xi_3\eta_1^2+\xi_2^2\xi_3^2]\right\},$$

$$I_{1,6,6} = -\mathrm{i}\zeta\sqrt{\frac{21}{26}}\left\{\frac{1}{8}[33\eta_1^5-30\xi_2\xi_3\eta_1^3+5\xi_2^2\xi_3^2\eta_1]\right\},$$

$$I_{1,7,7} = \mathrm{i}\zeta\sqrt{\frac{14}{15}}\left\{\frac{1}{64}[429\eta_1^6-495\xi_2\xi_3\eta_1^4 +135\xi_2^2\xi_3^2\eta_1^2-5\xi_2^3\xi_3^3]\right\},$$

$$I_{2,2,3} = \mathrm{i}\zeta3\sqrt{\frac{2}{35}}\left\{\frac{1}{4}[5\eta_1\eta_2-\xi_3\eta_3]\right\},$$

$$I_{2,3,4} = -\mathrm{i}\zeta\sqrt{\frac{5}{7}}\left\{\frac{1}{4}[7\eta_1^2\eta_2-\xi_2\xi_3\eta_2-2\xi_3\eta_1\eta_3]\right\},$$

$$I_{2,4,5} = \mathrm{i}\zeta\sqrt{\frac{10}{11}}\left\{\frac{1}{8}[21\eta_1^3\eta_2-7\xi_2\xi_3\eta_1\eta_2-7\xi_3\eta_1^2\eta_3 +\xi_2\xi_3^2\eta_3]\right\},$$

$$I_{2,5,6} = -\mathrm{i}\zeta3\sqrt{\frac{35}{286}}\left\{\frac{1}{8}[33\eta_1^4\eta_2-18\xi_2\xi_3\eta_1^2\eta_2 +\xi_2^2\xi_3^2\eta_2-12\xi_3\eta_1^3\eta_3+4\xi_2\xi_3^2\eta_1\eta_3]\right\},$$

$$I_{2,6,7} = \mathrm{i}\zeta2\sqrt{\frac{21}{65}}\left\{\frac{1}{64}[429\eta_1^5\eta_2-330\xi_2\xi_3\eta_1^3\eta_2 +45\xi_2^2\xi_3^2\eta_1\eta_2-165\xi_3\eta_1^4\eta_3+90\xi_2\xi_3^2\eta_1^2\eta_3 -5\xi_2^2\xi_3^3\eta_3]\right\},$$

$$I_{3,3,3} = -\mathrm{i}\zeta\sqrt{\frac{6}{7}}\left\{\frac{1}{12}[-5\xi_2\eta_2^2+25\eta_1\eta_2\eta_3-5\xi_3\eta_3^2 -5\xi_1\eta_1^2+2\xi_1\xi_2\xi_3]\right\},$$

$$I_{3,3,5} = \mathrm{i}\zeta5\sqrt{\frac{3}{77}}\left\{\frac{1}{24}[63\eta_1^2\eta_2^2-7\xi_2\xi_3\eta_2^2-28\xi_3\eta_1\eta_2\eta_3 +2\xi_3^2\eta_3^2-7\xi_1\xi_3\eta_1^2+\xi_1\xi_2\xi_3^2]\right\},$$

$$I_{3,4,4} = \mathrm{i}\zeta3\sqrt{\frac{10}{77}}\left\{\frac{1}{72}[-70\xi_2\eta_1\eta_2^2+245\eta_1^2\eta_2\eta_3 -15\xi_2\xi_3\eta_2\eta_3-70\xi_3\eta_1\eta_3^2-49\xi_1\eta_1^3+31\xi_1\xi_2\xi_3\eta_1]\right\},$$

$$I_{3,4,6} = -\mathrm{i}\zeta5\sqrt{\frac{7}{143}}\left\{\frac{1}{8}[33\eta_1^3\eta_2^2-9\xi_2\xi_3\eta_1\eta_2^2-18\xi_3\eta_1^2\eta_2\eta_3 +2\xi_2\xi_3^2\eta_2\eta_3+2\xi_3^2\eta_1\eta_3^2-3\xi_1\xi_3\eta_1^3+\xi_1\xi_2\xi_3^2\eta_1]\right\},$$

$$I_{3,5,5} = -\mathrm{i}\zeta\sqrt{\frac{210}{143}}\left\{\frac{1}{24}[-45\xi_2\eta_1^2\eta_2^2+5\xi_2^2\xi_3\eta_2^2+135\eta_1^3\eta_2\eta_3 -25\xi_2\xi_3\eta_1\eta_2\eta_3-45\xi_3\eta_1^2\eta_3^2+5\xi_2\xi_3^2\eta_3^2-27\xi_1\eta_1^4 +23\xi_1\xi_2\xi_3\eta_1^2-2\xi_1\xi_2^2\xi_3^2]\right\},$$

$$I_{3,5,7} = \mathrm{i}\zeta\sqrt{\frac{210}{143}}\left\{\frac{1}{64}[429\eta_1^4\eta_2^2-198\xi_2\xi_3\eta_1^2\eta_2^2+9\xi_2^2\xi_3^2\eta_2^2 -264\xi_3\eta_1^3\eta_2\eta_3+72\xi_2\xi_3^2\eta_1\eta_2\eta_3+36\xi_3^2\eta_1^2\eta_3^2 -4\xi_2\xi_3^3\eta_3^2-33\xi_1\xi_3\eta_1^4+18\xi_1\xi_2\xi_3^2\eta_1^2-\xi_1\xi_2^2\xi_3^3]\right\},$$

$$I_{4,4,5} = -\mathrm{i}\zeta\frac{15}{\sqrt{143}}\left\{\frac{1}{72}[-126\xi_2\eta_1\eta_2^3+441\eta_1^2\eta_2^2\eta_3$$

$$-7\xi_2\xi_3\eta_2^2\eta_3-196\xi_3\eta_1\eta_2\eta_3^2+14\xi_3^2\eta_3^3-126\xi_1\eta_1^3\eta_2$$
$$\left.+84\xi_1\xi_2\xi_3\eta_1\eta_2-7\xi_1\xi_3\eta_1^2\eta_3-5\xi_1\xi_2\xi_3^2\eta_3]\right\},$$

$$I_{4,4,7} = \mathrm{i}\zeta\frac{14}{3}\sqrt{\frac{10}{143}}\left\{\frac{1}{64}[429\eta_1^3\eta_2^3-99\xi_2\xi_3\eta_1\eta_2^3\right.$$
$$-297\xi_3\eta_1^2\eta_2^2\eta_3+27\xi_2\xi_3^2\eta_2^2\eta_3+54\xi_3^2\eta_1\eta_2\eta_3^2$$
$$-2\xi_3^3\eta_3^3-99\xi_1\xi_3\eta_1^3\eta_2+27\xi_1\xi_2\xi_3^2\eta_1\eta_2$$
$$\left.+27\xi_1\xi_3^2\eta_1^2\eta_3-3\xi_1\xi_2\xi_3^3\eta_3]\right\}.$$

5 Conclusions

The rotational invariants $I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ constructed by three spherical harmonic polynomials are the homogeneous polynomials of orders j, k, and ℓ with respect to the three coordinate vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$, respectively. We have rewritten the definitions for the invariants given by Biedenharn and Louck more explicitly, derived the recursive relations for the coefficients A_{abc} and B_{abc} using the Laplace's equations, defined two key functions $G_{a,b}$ and $F_{a,b}$ in (21) and (31), and calculated analytically the expressions for A_{abc} and B_{abc} by mathematical induction, as given in (22–24) and (32–34). Therefore, we have completely solved the problem raised by Biedenharn and Louck (p.308 of Ref. [2]). The present method can in principle be generalized to the rotational invariants constructed by four or more spherical harmonic polynomials although the definition for the invariants depends on the order of coupling.

MA Zhong-Qi would like to thank Professor Zhang Fu-Chun for the warm hospitality during his visit at the University of Hong Kong where part of this work was completed.

Appendix A

Invariants calculated from their definitions

Choosing a special rotation such that $\boldsymbol{r}_1$ is along the z axis and $\boldsymbol{r}_2$ is in the xz plane with x positive, we have

$$\mathcal{Y}^j_\mu(\boldsymbol{r}_1) = \mathcal{Y}^j_\mu(\xi_1^{1/2},0,0)=\sqrt{\frac{(2j+1)\xi_1^j}{4\pi}}\delta_{\mu 0},$$

$$\mathcal{Y}^k_\nu(\boldsymbol{r}_2) = \mathcal{Y}^k_\nu(\xi_2^{1/2},\theta_{12},0)$$
$$= (-1)^{(\nu+|\nu|)/2}\left[\frac{(2k+1)\xi_2^k(k-|\nu|)!(k+|\nu|)!}{4\pi 4^{|\nu|}(k!)^2}\right]^{1/2}$$
$$\times(\sin\theta_{12})^{|\nu|}P^{(|\nu|,|\nu|)}_{k-|\nu|}(\cos\theta_{12}),$$

$$\mathcal{Y}^\ell_{-\nu}(\boldsymbol{r}_3) = \mathcal{Y}^\ell_{-\nu}(\xi_3^{1/2},\theta_{13},\varphi)$$
$$= (-1)^{(-\nu+|\nu|)/2}\left[\frac{(2\ell+1)\xi_3^\ell(\ell-|\nu|)!(\ell+|\nu|)!}{4\pi 4^{|\nu|}(\ell!)^2}\right]^{1/2}$$
$$\times(\sin\theta_{13})^{|\nu|}P^{(|\nu|,|\nu|)}_{\ell-|\nu|}(\cos\theta_{13})\mathrm{e}^{-\mathrm{i}\nu\varphi},$$

where $P_n^{(\alpha,\beta)}$ is the Jacobi's polynomial (see 8.960 in Ref. [15])

$$P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n}\sum_{m=0}^{n}\begin{pmatrix} n+\alpha \\ m\end{pmatrix}\begin{pmatrix} n+\beta \\ n-m\end{pmatrix}$$
$$\times(x-1)^{n-m}(x+1)^m,$$

and the angles satisfy

$$\cos\theta_{ab} = \sum_{c=1}^{3}\epsilon_{abc}\eta_c(\xi_a\xi_b)^{-1/2},$$

$$\cos\varphi = \frac{\cos\theta_{23}-\cos\theta_{12}\cos\theta_{13}}{\sin\theta_{12}\sin\theta_{13}},$$

$$\zeta = (\xi_1\xi_2\xi_3)^{1/2}\sin\theta_{12}\sin\theta_{13}\sin\varphi.$$

Thus,

$$I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$$
$$= \frac{\sqrt{\xi_1^j\xi_2^k\xi_3^\ell}}{k!\ell!}\sum_{\nu=-k}^{k}(-1)^\nu\begin{pmatrix} j & k & \ell \\ 0 & \nu & -\nu\end{pmatrix}$$
$$\times\frac{\sqrt{(k-\nu)!(k+\nu)!(\ell-\nu)!(\ell+\nu)!}}{4^{|\nu|}}(\sin\theta_{12}\sin\theta_{13})^{|\nu|}$$
$$\times P^{(|\nu|,|\nu|)}_{k-|\nu|}(\cos\theta_{12})P^{(|\nu|,|\nu|)}_{\ell-|\nu|}(\cos\theta_{13})\mathrm{e}^{-\mathrm{i}\nu\varphi}. \qquad (\mathrm{A1})$$

From the identity

$$\cos(\nu\varphi)+\mathrm{i}\sin(\nu\varphi)$$
$$= \mathrm{e}^{\mathrm{i}\nu\varphi}=[\cos\varphi+\mathrm{i}\sin\varphi]^\nu$$
$$= \sum_{r=0}^{\nu}\begin{pmatrix}\nu \\ r\end{pmatrix}(\cos\varphi)^{\nu-r}(\mathrm{i}\sin\varphi)^r,$$

one obtains for $\nu\geqslant 0$

$$\cos\nu\varphi = \sum_{r=0}^{[\nu/2]}\sum_{s=0}^{r}(-1)^{r+s}\begin{pmatrix}\nu\\2r\end{pmatrix}\begin{pmatrix}r\\s\end{pmatrix}(\cos\varphi)^{\nu-2r+2s},$$

$$\sin\nu\varphi = \sin\varphi\sum_{r=0}^{[(\nu-1)/2]}\sum_{s=0}^{r}(-1)^{r+s}\begin{pmatrix}\nu\\2r+1\end{pmatrix}\times\begin{pmatrix}r\\s\end{pmatrix}(\cos\varphi)^{\nu-1-2r+2s}.$$

Substituting them into (A1), we obtain

$$\begin{aligned}&I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)\\&=\frac{\sqrt{\xi_1^j\xi_2^k\xi_3^\ell}}{k!\ell!}\sum_{\nu=-k}^{k}(-1)^\nu\begin{pmatrix}j&k&\ell\\0&\nu&-\nu\end{pmatrix}\\&\times\frac{\sqrt{(k-\nu)!(k+\nu)!(\ell-\nu)!(\ell+\nu)!}}{4^{|\nu|}}P_{k-|\nu|}^{(|\nu|,|\nu|)}(\cos\theta_{12})\\&\times P_{\ell-|\nu|}^{(|\nu|,|\nu|)}(\cos\theta_{13})\sum_{r=0}^{[|\nu|/2]}\sum_{s=0}^{r}(-1)^{r+s}\begin{pmatrix}|\nu|\\2r\end{pmatrix}\begin{pmatrix}r\\s\end{pmatrix}\\&\times(\cos\theta_{23}-\cos\theta_{12}\cos\theta_{13})^{|\nu|-2r+2s}\\&\times\left[\left(1-\cos^2\theta_{12}\right)\left(1-\cos^2\theta_{13}\right)\right]^{r-s},\end{aligned}\tag{A2}$$

for even $j+k+\ell$, and

$$\begin{aligned}&I_{j,k,\ell}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)\\&=-\mathrm{i}\zeta\frac{\sqrt{\xi_1^{j-1}\xi_2^{k-1}\xi_3^{\ell-1}}}{k!\ell!}\sum_{\nu=-k}^{k}(-1)^\nu\mathrm{sign}(\nu)\\&\times\begin{pmatrix}j&k&\ell\\0&\nu&-\nu\end{pmatrix}\frac{\sqrt{(k-\nu)!(k+\nu)!(\ell-\nu)!(\ell+\nu)!}}{4^{|\nu|}}\\&\times P_{k-|\nu|}^{(|\nu|,|\nu|)}(\cos\theta_{12})P_{\ell-|\nu|}^{(|\nu|,|\nu|)}(\cos\theta_{13})\\&\times\sum_{r=0}^{[(|\nu|-1)/2]}\sum_{s=0}^{r}(-1)^{r+s}\begin{pmatrix}|\nu|\\2r+1\end{pmatrix}\begin{pmatrix}r\\s\end{pmatrix}\\&\times(\cos\theta_{23}-\cos\theta_{12}\cos\theta_{13})^{|\nu|-1-2r+2s}\\&\times\left[\left(1-\cos^2\theta_{12}\right)\left(1-\cos^2\theta_{13}\right)\right]^{r-s}.\end{aligned}\tag{A3}$$

for odd $j+k+\ell$.

References

1 Weyl H. The Classical Groups: Their Invariants and Representations. Princeton, New Jersey: Princeton University Press, 1946

2 Biedenharn L C, Louck J D. The Racah-Wigner Algebra in Quantum Theory, Encyclopedia of Mathematics and its Application. Vol. 9. Ed. Rota G C. Massachusetts: Addison-Wesley, 1981

3 Fromm D M, Hill R N. Phys. Rev. A, 1987, **36**: 1013

4 Harris F E. Integrals for Exponentially Correlated Four-body Systems of General Angular Symmetry. Vol. III, Ed. Brändas E J, Kryachko E S. Fundamental World of Quantum Chemistry, Dordrecht, Kluwer, 2004. 115

5 Manakov N L, Marmo S I, Meremianin A V. J. Phys. B, 1996, **29**: 2711

6 Manakov N L, Meremianin A V, Starace A F. Phys. Rev. A, 1998, **57**: 3233

7 Meremianin A V, Briggs J S. Phys. Rep., 2003, **384**: 121

8 Borisenko O, Kushnir V. Ukr. J. Phys., 2006, **51**: N 1, 90

9 Joshi N, Jhingan S, Souradeep T, Hajian A. Phys. Rev. D, 2010, **81**: 083012

10 Rocha G, Hobson M P, Smith S, Ferreira P, Challinor A. Mon. Not. R. Astron. Soc., 2005, **357**: 1

11 Pápai P, Szapudi I. Mon. Not. R. Astron. Soc., 2008, **389**: 292

12 Raccanelli A, Samushia L, Percival W J. Mon. Not. R. Astron. Soc., 2010, **409**: 1525

13 GU X Y, DUAN B, MA Z Q. Phys. Rev. A, 2001, **64**: 042108

14 MA Z Q. Group Theory for Physicists. Singapore: World Scientific, 2007

15 Gradshteyn I S, Ryzhik I M. Table of Integrals, Series, and Products. Ed. Jeffrey A, Zwillinger D. 7th Ed. Academic Press, 2007