



HAL
open science

The orthogonal group action on spatial vectors: invariants, covariants, and syzygies

Guillaume Dhont, Patrick Cassam-Chenaï, Boris Zhilinskii, Frédéric Patras

► To cite this version:

Guillaume Dhont, Patrick Cassam-Chenaï, Boris Zhilinskii, Frédéric Patras. The orthogonal group action on spatial vectors: invariants, covariants, and syzygies. 2015. hal-01222972v1

HAL Id: hal-01222972

<https://hal.science/hal-01222972v1>

Preprint submitted on 31 Oct 2015 (v1), last revised 7 Sep 2021 (v5)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Version: today is 31 October 2015.

The orthogonal group action on spatial vectors: invariants, covariants, and syzygies

Guillaume Dhont¹, Boris I Zhilinskiĭ¹, Patrick Cassam-Chenaï²
and Frédéric Patras²

¹ Université du Littoral Côte d'Opale, Laboratoire de Physico-Chimie de
l'Atmosphère, MREI2, 189A avenue Maurice Schumann, 59140 Dunkerque, France

² Laboratoire J. A. Dieudonné, Université de Nice-Sophia Antipolis, Parc Valrose,
06100 Nice, France

E-mail: guillaume.dhont@univ-littoral.fr

Abstract. The present paper on the $SO(3)$ invariants and covariants built from N vectors of the three-dimensional space is the follow-up of our previous article [1] dealing with planar vectors and $SO(2)$ symmetry.

The goal is to propose integrity basis for the set of $SO(3)$ invariants and covariant free modules and easy-to-use generating families in the case of non-free covariants modules. The existence of such non-free modules is one of the noteworthy features unseen when dealing with finite point groups, that we want to point out. As in paper [1], the Molien function plays a central role in the conception of these bases. The Molien functions are computed and checked by the use of two independent paths. The first computation relies on the Molien integral [2] and requires the matrix representation of the group action on the N spatial vectors. The second path considers the Molien function for only one spatial vector as the elementary building material from which are worked out the other Molien functions.

PACS numbers: 02.20.-a, 02.20.Hj, 31.15.xh, 31.30.jy, 33.20.Vq

AMS classification scheme numbers: 13A50, 15A72, 16W22

Submitted to: *J. Phys. A: Math. Gen.*

1. Introduction

The present paper on the $\text{SO}(3)$ invariants and covariants built from N vectors of the three-dimensional space is the follow-up of our previous article [1] dealing with planar vectors and $\text{SO}(2)$ symmetry.

The goal is to propose integrity basis for the set of $\text{SO}(3)$ invariants and covariant free modules and easy-to-use generating families in the case of non-free covariants modules. The existence of such non-free modules is one of the noteworthy features unseen when dealing with finite point groups, that we want to point out. As in paper [1], the Molien function plays a central role in the conception of these bases. The Molien functions are computed and checked by the use of two independent paths. The first computation relies on the Molien integral [2] and requires the matrix representation of the group action on the N spatial vectors. The second path considers the Molien function for only one spatial vector as the elementary building material from which are worked out the other Molien functions.

2. Construction of the generating function for N vectors

2.1. Molien integral

2.1.1. Parametrization A rotation of a point M that leaves invariant the origin O of the three-dimensional space can be described as a rotation of angle ω around a rotation axis whose position is defined through the θ and φ spherical angles with respect to the $(Ox_1y_1z_1)$ system of axes, see Figure 1. As usual, the spherical angles are defined to be in the $0 \leq \theta \leq \pi$ and $0 \leq \varphi < 2\pi$ intervals. A rotation with a negative angle of rotation $\omega < 0$ around the rotation axis with (θ, φ) spherical coordinates is equivalent to a rotation with the opposite angle of rotation $-\omega > 0$ and the opposite axis of rotation with $(\pi - \theta, \varphi + \pi)$ spherical coordinates. The $0 \leq \omega \leq \pi$ interval of rotation angle is enough to cover all possible rotations. This parametrization counts twice the rotations with a rotation angle $\omega = \pi$ (a rotation of π around the rotation axis with $(\pi - \theta, \varphi + \pi)$ spherical angles is identical to a rotation of π around the rotation axis with (θ, φ) spherical angles) but this is a set of measure zero.

2.1.2. Definition of a basis vector attached to the rotation axis We construct a basis vector attached to the rotation axis whose vectors $\vec{e}_{x_3}, \vec{e}_{y_3}, \vec{e}_{z_3}$ are deduced from the initial basis vector $\vec{e}_{x_1}, \vec{e}_{y_1}, \vec{e}_{z_1}$ through two successive rotations of the axes such that the rotation axis coincides with the Oz_3 axis, see Figure 2:

step 1: rotation of the axes by an angle φ around the z_1 axis:

$$\begin{pmatrix} \vec{e}_{x_2} & \vec{e}_{y_2} & \vec{e}_{z_2} \end{pmatrix} = \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (1)$$

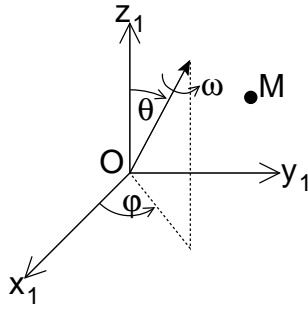


Figure 1. Parametrization of a rotation in three-dimensional space. The θ and φ angles are the spherical angles of the rotation axis, the ω angle is the rotation angle around the rotation axis.

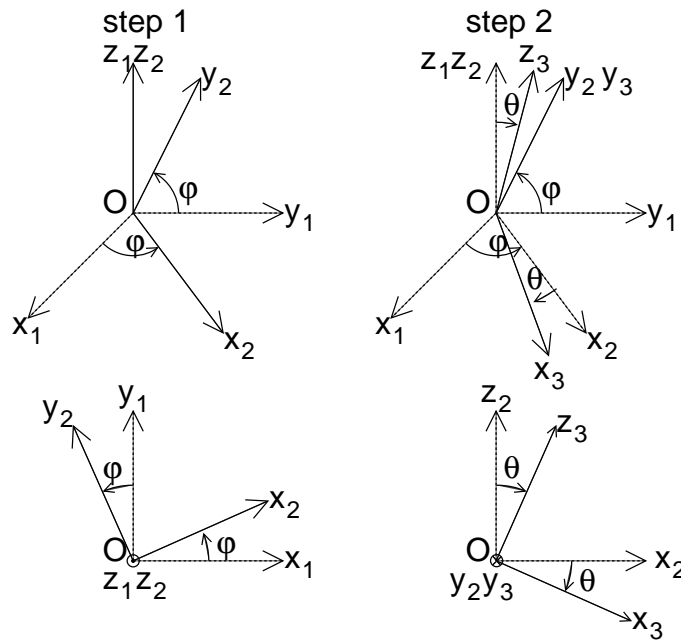


Figure 2. Definition of the $(Ox_3y_3z_3)$ frame.

step 2: rotation of the axes by an angle θ around the y_2 axis:

$$\begin{pmatrix} \vec{e}_{x_3} & \vec{e}_{y_3} & \vec{e}_{z_3} \end{pmatrix} = \begin{pmatrix} \vec{e}_{x_2} & \vec{e}_{y_2} & \vec{e}_{z_2} \end{pmatrix} \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}. \quad (2)$$

The relation between the initial basis $\vec{e}_{x_1}, \vec{e}_{y_1}, \vec{e}_{z_1}$ and the final basis $\vec{e}_{x_3}, \vec{e}_{y_3}, \vec{e}_{z_3}$ is then:

$$\begin{pmatrix} \vec{e}_{x_3} & \vec{e}_{y_3} & \vec{e}_{z_3} \end{pmatrix} = \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}$$

$$= \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \underbrace{\begin{pmatrix} \cos \varphi \cos \theta & -\sin \varphi & \cos \varphi \sin \theta \\ \sin \varphi \cos \theta & \cos \varphi & \sin \varphi \sin \theta \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}}_{=M_1(\theta, \varphi)}. \quad (3)$$

The matrix $M_1(\theta, \varphi)$ is an orthogonal matrix:

$$M_1(\theta, \varphi) M_1(\theta, \varphi)^T = M_1(\theta, \varphi)^T M_1(\theta, \varphi) = I_{3 \times 3}.$$

2.1.3. *Rotation of the point M in $(Ox_3y_3z_3)$* It is easy to describe the rotation of a point M around the z_3 axis by an angle ω , see Figure 3:

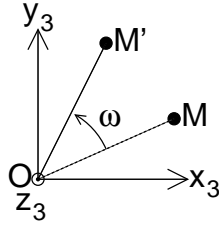


Figure 3. Rotation of point M in the $(Ox_3y_3z_3)$ frame.

$$\begin{pmatrix} x'_3 \\ y'_3 \\ z'_3 \end{pmatrix} = \underbrace{\begin{pmatrix} \cos \omega & -\sin \omega & 0 \\ \sin \omega & \cos \omega & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{=M_2(\omega)} \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \quad (4)$$

2.1.4. *Rotation of the point M in $(Ox_1y_1z_1)$* Let x_1, y_1, z_1 and x_3, y_3, z_3 be the coordinates of point M respectively in the $(Ox_1y_1z_1)$ and $(Ox_3y_3z_3)$ system of axes:

$$\overrightarrow{OM} = x_1 \vec{e}_{x_1} + y_1 \vec{e}_{y_1} + z_1 \vec{e}_{z_1} = x_3 \vec{e}_{x_3} + y_3 \vec{e}_{y_3} + z_3 \vec{e}_{z_3}. \quad (5)$$

Relation (5) can be written as:

$$\begin{aligned} \overrightarrow{OM} &= \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} \\ &= \begin{pmatrix} \vec{e}_{x_3} & \vec{e}_{y_3} & \vec{e}_{z_3} \end{pmatrix} \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \\ &= \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} M_1(\theta, \varphi) \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \end{aligned} \quad (6)$$

We deduce from (6) the relation between x_1, y_1, z_1 and x_3, y_3, z_3 :

$$\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = M_1(\theta, \varphi) \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix}, \quad (7)$$

$$\begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} = M_1(\theta, \varphi)^T \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}. \quad (8)$$

The primed variables are the coordinates for $\overrightarrow{OM'}$:

$$\overrightarrow{OM'} = x'_1 \vec{e}_{x_1} + y'_1 \vec{e}_{y_1} + z'_1 \vec{e}_{z_1} = x'_3 \vec{e}_{x_3} + y'_3 \vec{e}_{y_3} + z'_3 \vec{e}_{z_3}. \quad (9)$$

Finally, we obtain that:

$$\begin{aligned} \begin{pmatrix} x'_1 \\ y'_1 \\ z'_1 \end{pmatrix} &= M_1(\theta, \varphi) \begin{pmatrix} x'_3 \\ y'_3 \\ z'_3 \end{pmatrix} \\ &= M_1(\theta, \varphi) M_2(\omega) \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \\ \begin{pmatrix} x'_1 \\ y'_1 \\ z'_1 \end{pmatrix} &= M_1(\theta, \varphi) M_2(\omega) M_1(\theta, \varphi)^T \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} \end{aligned} \quad (10)$$

The rotation matrix $M(\varphi, \theta, \omega)$ is

$$M(\varphi, \theta, \omega) = M_1(\theta, \varphi) M_2(\omega) M_1(\theta, \varphi)^T. \quad (11)$$

2.1.5. Molien function Invariant integral:

$$\int_0^\pi \int_0^{2\pi} \int_0^\pi f(\varphi, \theta, \omega) \sin \theta d\theta d\varphi \sin^2 \frac{\omega}{2} d\omega.$$

Normalization factor:

$$\int_0^\pi \int_0^{2\pi} \int_0^\pi \sin \theta d\theta d\varphi \sin^2 \frac{\omega}{2} d\omega = 4\pi \frac{\pi}{2} = 2\pi^2.$$

Each rotation angle defines a class, all the rotations with the same angle but different rotation axes belong to the same class. The character $\chi^{(L)}$ is equal to:

$$\chi^{(L)}(\omega) = \frac{\sin\left(L + \frac{1}{2}\right)\omega}{\sin \frac{\omega}{2}}.$$

The Molien function for computing the number of invariants or covariants of representation (L) , $L \in \mathbb{N}$ from N space vectors \overrightarrow{OM}_i is given by

$$\frac{1}{2\pi^2} \int_0^\pi \int_0^{2\pi} \int_0^\pi \frac{\chi^{(L)}(\omega)^*}{\det(I - \lambda D(\varphi, \theta, \omega))} \sin \theta d\theta d\varphi \sin^2 \frac{\omega}{2} d\omega \quad (12)$$

where $D(\varphi, \theta, \omega)$ is a $3N \times 3N$ block matrix representation of the rotation operation:

$$D(\varphi, \theta, \omega) = \begin{pmatrix} M(\varphi, \theta, \omega) & 0 & \cdots & 0 \\ 0 & M(\varphi, \theta, \omega) & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & M(\varphi, \theta, \omega) \end{pmatrix}$$

We find that

$$\det(I - \lambda D(\varphi, \theta, \omega)) = [(1 - \lambda)(1 - 2\lambda \cos \omega + \lambda^2)]^N. \quad (13)$$

2.1.6. Generating functions for the invariants

$$\begin{aligned} & g_{\text{Molien}}^{\text{SO}(3)}(\Gamma_{\text{final}} = (0); \Gamma_N; \lambda) \\ &= \frac{1}{2\pi^2} \int_0^\pi \int_0^{2\pi} \int_0^\pi \frac{1}{[(1 - \lambda)(1 - 2\lambda \cos \omega + \lambda^2)]^N} \sin \theta d\theta d\varphi \sin^2 \frac{\omega}{2} d\omega \\ &= \frac{2}{\pi} \frac{1}{(1 - \lambda)^N} \int_0^\pi \frac{\sin^2 \frac{\omega}{2}}{(1 - 2\lambda \cos \omega + \lambda^2)^N} d\omega \end{aligned} \quad (14)$$

2.1.7. Generating functions for the (L) covariants

$$\begin{aligned} & g_{\text{Molien}}^{\text{SO}(3)}(\Gamma_{\text{final}} = (L); \Gamma_N; \lambda) \\ &= \frac{1}{2\pi^2} \int_0^\pi \int_0^{2\pi} \int_0^\pi \frac{\frac{\sin(L + \frac{1}{2})\omega}{\sin \frac{\omega}{2}}}{[(1 - \lambda)(1 - 2\lambda \cos \omega + \lambda^2)]^N} \sin \theta d\theta d\varphi \sin^2 \frac{\omega}{2} d\omega \\ &= \frac{2}{\pi} \frac{1}{(1 - \lambda)^N} \int_0^\pi \frac{[\sin(L + \frac{1}{2})\omega] \sin \frac{\omega}{2}}{(1 - 2\lambda \cos \omega + \lambda^2)^N} d\omega \end{aligned} \quad (15)$$

Remark:

$$\left[\sin\left(L + \frac{1}{2}\right)\omega \right] \sin \frac{\omega}{2} = \frac{\cos(L\omega) - \cos[(L + 1)\omega]}{2}$$

$$\begin{aligned} & g_{\text{Molien}}^{\text{SO}(3)}(\Gamma_{\text{final}} = (L); \Gamma_N; \lambda) \\ &= \frac{1}{(1 - \lambda)^N} \left\{ \frac{1}{\pi} \int_0^\pi \frac{\cos(L\omega) d\omega}{(1 - 2\lambda \cos \omega + \lambda^2)^N} - \frac{1}{\pi} \int_0^\pi \frac{\cos[(L + 1)\omega] d\omega}{(1 - 2\lambda \cos \omega + \lambda^2)^N} \right\} \\ &= \frac{1}{(1 - \lambda)^N} \left(g_{\text{Molien}}^{\text{SO}(2)}(\Gamma_{\text{final}} = (L); \Gamma_N; \lambda) - g_{\text{Molien}}^{\text{SO}(2)}(\Gamma_{\text{final}} = (L + 1); \Gamma_N; \lambda) \right) \end{aligned} \quad (16)$$

From [3],

$$\int_0^\pi \frac{\cos nx \, dx}{(1 - 2a \cos x + a^2)^m} = \begin{cases} \frac{a^{2m+n-2}\pi}{(1-a^2)^{2m-1}} \sum_{k=0}^{m-1} \binom{m+n-1}{k} \binom{2m-k-2}{m-1} \left(\frac{1-a^2}{a^2}\right)^k & [a^2 < 1] \\ \frac{\pi}{a^n(a^2-1)^{2m-1}} \sum_{k=0}^{m-1} \binom{m+n-1}{k} \binom{2m-k-2}{m-1} (a^2-1)^k & [a^2 > 1] \end{cases}$$

Remark: Collins and Parsons [4] compute the Molien function for the invariants using the Euler angle parametrization of the rotations. The numerator in the integrand of the Molien function is just 1 for the invariant and both parametrization (ours and theirs) are equivalent. For covariants, the numerator in the integrand is the character which depends only on rotation angle. For covariant, our parametrization gives a straightforward integral over only one variable ω while calculations would not be so direct using Euler angles. It perhaps may be done using the remark page 488 of [5] :

Using explicit expressions for the rotation matrix elements and Eq. (B30), we find a simple relation between the rotation angle δ about an arbitrary axis and the Euler angles:

$$\cos\left(\frac{\delta}{2}\right) = \cos\left[\frac{\alpha + \beta}{2}\right] \cos\left(\frac{\beta}{2}\right).$$

3. One spatial vector

$$g_1^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_1^{\text{SO}(3)}; \lambda\right) = \frac{\lambda^L}{1 - \lambda^2}. \quad (17)$$

The initial representation Γ_1 contains the three variables x_1, y_1, z_1 , and the sum over L of $(2L + 1) g_1^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_1^{\text{SO}(3)}; \lambda\right)$ is equal to $\frac{1}{(1-\lambda)^3}$:

$$\sum_{L=0}^{\infty} (2L + 1) g_1^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_1^{\text{SO}(3)}; \lambda\right) = \frac{1}{(1 - \lambda)^3}.$$

What are the polynomials of lowest degrees?

$$\begin{aligned} & \frac{1}{(1 - \lambda)^3} \\ &= (1 + \lambda + \lambda^2 + \lambda^3 + \dots) (1 + \lambda + \lambda^2 + \lambda^3 + \dots) (1 + \lambda + \lambda^2 + \lambda^3 + \dots) \\ &= 1 + 3\lambda + 6\lambda^2 + 10\lambda^3 + \dots \end{aligned}$$

See Table 1.

Table 1. Polynomials of degree n built from representation $(1)^{\text{SO}(3)}$.

n	$\binom{3+n-1}{n}$	polynomials
0	1	1
1	3	x, y, z
2	$\frac{4!}{2!2!} = 6$	$x^2, y^2, z^2, xy, xz, yz$
3	$\frac{5!}{3!2!} = 10$	$x^3, y^3, z^3, x^2y, x^2z, xy^2, y^2z, xz^2, yz^2, xyz$

4. Two spatial vectors

The six coordinates $\{x_1, y_1, z_1, x_2, y_2, z_2\}$ of the two spatial vectors span a six-dimensional reducible representation: $\{x_1, y_1, z_1, x_2, y_2, z_2\}$ and is reducible: $\Gamma_2^{\text{SO}(3)} = \Gamma_1^{\text{SO}(3)} \oplus \Gamma_1^{\text{SO}(3)}$. The generating functions for two vectors can be deduced by coupling the generating functions for one vector obtained in (3), see Appendix A.

$$g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_2^{\text{SO}(3)}; \lambda \right) = \frac{(L+1)\lambda^L + L\lambda^{L+1}}{(1-\lambda^2)^3}. \quad (18)$$

The ring of invariant is well-known [6] and generated by the 3 scalar products: $Q_1 = x_1^2 + y_1^2 + z_1^2$, $Q_2 = x_2^2 + y_2^2 + z_2^2$, $Q_3 = x_1x_2 + y_1y_2 + z_1z_2$.

For $L = 1$,

$$g_1^{\text{SO}(3)} \left((1); \Gamma_2^{\text{SO}(3)}; \lambda \right) = \frac{2\lambda + \lambda^2}{(1-\lambda^2)^3}. \quad (19)$$

The two first order (1)-covariant basis vectors can be taken as $\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$ and $\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$, and

the second order one as their cross-product $\begin{pmatrix} y_1z_2 - z_1y_2 \\ z_1x_2 - x_2z_1 \\ x_1y_2 - y_1x_2 \end{pmatrix}$.

So the z-component of the electric dipole moment function of an ABC molecule will have the form:

$$DMS[x_1, y_1, z_1, x_2, y_2, z_2] = P_{z_1}[Q_1, Q_2, Q_3]z_1 + P_{z_2}[Q_1, Q_2, Q_3]z_2 + P_{x_1y_2 - y_1x_2}[Q_1, Q_2, Q_3](x_1y_2 - y_1x_2), \quad (20)$$

where P_i are polynomials in the primary invariants. The other components are related by symmetry which implies $P_{x_i} = P_{y_i} = P_{z_i}$ and $P_{y_1z_2 - z_1y_2} = P_{z_1x_2 - x_1z_2} = P_{x_1y_2 - y_1x_2}$. So, only three polynomials in three variables need to be fitted on data to determine the DMS functions.

For $L = 2$,

$$g_1^{\text{SO}(3)} \left((2); \Gamma_2^{\text{SO}(3)}; \lambda \right) = \frac{3\lambda^2 + 2\lambda^3}{(1 - \lambda^2)^3}. \quad (21)$$

The three second order (2)-covariant basis vectors can be taken (probably?) as
 $\begin{pmatrix} 2z_1^2 - x_1^2 - y_1^2 \\ x_1z_1 \\ y_1z_1 \\ x_1y_1 \\ x_1^2 - y_1^2 \end{pmatrix}, \begin{pmatrix} 2z_2^2 - x_2^2 - y_2^2 \\ x_2z_2 \\ y_2z_2 \\ x_2y_2 \\ x_2^2 - y_2^2 \end{pmatrix}$ and $\begin{pmatrix} 2z_1z_2 - x_1x_2 - y_1y_2 \\ x_1z_2 + x_2z_1 \\ y_1z_2 + z_1y_2 \\ x_1y_2 + y_1x_2 \\ x_1x_2 - y_1y_2 \end{pmatrix}$, and the third order ones as ...

5. Three spatial vectors

The initial representation $\Gamma_3^{\text{SO}(3)} = \Gamma_1^{\text{SO}(3)} \oplus \Gamma_1^{\text{SO}(3)} \oplus \Gamma_1^{\text{SO}(3)}$ contains nine variables and is reducible.

The generating functions for three vectors can be obtained by coupling the generating function for one vector and the generating function for two vectors, see Appendix Appendix A.

$$\begin{aligned} & g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_3^{\text{SO}(3)}; \lambda \right) \\ &= \frac{\frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} - (L+1)(L-1)\lambda^{L+3} - \frac{L(L-1)}{2}\lambda^{L+4}}{(1 - \lambda^2)^6}, \end{aligned} \quad (22)$$

$$\begin{aligned} & g_2^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_3^{\text{SO}(3)}; \lambda \right) \\ &= \frac{(2L+1)\lambda^L + (2L+1)\lambda^{L+1}}{(1 - \lambda^2)^6} \\ &+ \frac{\frac{L(L-1)}{2}\lambda^L + (L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}}{(1 - \lambda^2)^5}, \end{aligned} \quad (23)$$

The coefficients in (22) are greater or equal to zero if $L = 0$ or $L = 1$. Negative coefficients appear for $L \geq 2$, however the Molien function can be rewritten as (23). where all the coefficients in the numerators are positive coefficients for $L \geq 2$.

The generating function suitable for a symbolic interpretation in term of an integrity basis depends on L . Table 2 gives ...

6. Generating function for four vectors

$$\begin{aligned} & g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\ &= \frac{\mathcal{N} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right)}{(1 - \lambda^2)^9}, \end{aligned} \quad (24)$$

Table 2. Expressions of the $g_i^{\text{SO}(3)}$ Molien functions for three spatial vectors and the final $(L)^{\text{SO}(3)}$, $0 \leq L \leq 6$ irreducible representations.

i	$\Gamma_{\text{final}}^{\text{SO}(3)}$	$g_i^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_3^{\text{SO}(3)}; \lambda \right)$
1	(0)	$\frac{1+\lambda^3}{(1-\lambda^2)^6}$
1,2	(1)	$\frac{3\lambda+3\lambda^2}{(1-\lambda^2)^6}$
2	(2)	$\frac{5\lambda^2+5\lambda^3}{(1-\lambda^2)^6} + \frac{\lambda^2+3\lambda^3+\lambda^4}{(1-\lambda^2)^5}$
2	(3)	$\frac{7\lambda^3+7\lambda^4}{(1-\lambda^2)^6} + \frac{3\lambda^3+8\lambda^4+3\lambda^5}{(1-\lambda^2)^5}$
2	(4)	$\frac{9\lambda^4+9\lambda^5}{(1-\lambda^2)^6} + \frac{6\lambda^4+15\lambda^5+6\lambda^6}{(1-\lambda^2)^5}$
2	(5)	$\frac{11\lambda^5+11\lambda^6}{(1-\lambda^2)^6} + \frac{10\lambda^5+24\lambda^6+10\lambda^7}{(1-\lambda^2)^5}$
2	(6)	$\frac{13\lambda^6+13\lambda^7}{(1-\lambda^2)^6} + \frac{15\lambda^6+35\lambda^7+15\lambda^8}{(1-\lambda^2)^5}$
2	\vdots	\vdots

$$\begin{aligned}
 & \mathcal{N} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{(L+3)(L+2)(L+1)}{6} \lambda^L + \frac{(L+3)(L+2)L}{2} \lambda^{L+1} \\
 &+ \frac{(L+3)(L+2)(L+1)}{6} \lambda^{L+2} - \frac{(L+3)(L-2)(5L+4)}{6} \lambda^{L+3} \\
 &- \frac{(L+3)(L-2)(5L+1)}{6} \lambda^{L+4} + \frac{L(L-1)(L-2)}{6} \lambda^{L+5} \\
 &+ \frac{(L+1)(L-1)(L-2)}{2} \lambda^{L+6} + \frac{L(L-1)(L-2)}{6} \lambda^{L+7} \\
 &g_2^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{(L+3)(L+2)(L+1) \lambda^L + 4(2L+1) \lambda^{L+1} + (-\frac{1}{6}L^3 - L^2 + \frac{37}{6}L + 3) \lambda^{L+2}}{(1-\lambda^2)^9} \\
 &+ \frac{2(L-2)(2L+1) \lambda^{L+1} - \frac{(L-2)(L^2-16L-9)}{6} \lambda^{L+2}}{(1-\lambda^2)^8} \\
 &+ \frac{\frac{L(L-1)(L-2)}{2} \lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2} \lambda^{L+2} + \frac{L(L-1)(L-2)}{6} \lambda^{L+3}}{(1-\lambda^2)^7} \tag{25}
 \end{aligned}$$

$$\begin{aligned}
 & g_3^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{4(2L+1) \lambda^L + 4(2L+1) \lambda^{L+1}}{(1-\lambda^2)^9} \\
 &+ \frac{(\frac{1}{6}L^3 + L^2 - \frac{37}{6}L - 3) \lambda^L + 2(L-2)(2L+1) \lambda^{L+1} - \frac{(L-2)(L^2-16L-9)}{6} \lambda^{L+2}}{(1-\lambda^2)^8} \\
 &+ \frac{\frac{L(L-1)(L-2)}{2} \lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2} \lambda^{L+2} + \frac{L(L-1)(L-2)}{6} \lambda^{L+3}}{(1-\lambda^2)^7} \tag{26}
 \end{aligned}$$

$$g_4^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right)$$

$$\begin{aligned}
 &= \frac{4(2L+1)\lambda^L + 4(2L+1)\lambda^{L+1}}{(1-\lambda^2)^9} \\
 &+ \frac{2(L-3)(2L+1)\lambda^L + 2(L-2)(2L+1)\lambda^{L+1}}{(1-\lambda^2)^8} \\
 &+ \frac{\frac{(L-2)(L^2-16L-9)}{6}\lambda^L + \frac{L(L-1)(L-2)}{2}\lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}}{(1-\lambda^2)^7}
 \end{aligned} \tag{27}$$

The generating function (24) has positive or null coefficients in its numerators for $L = 0, 1$ or 2 .

Table 3. Expressions of the $g_i^{\text{SO}(3)}$ Molien functions for four spatial vectors and the final $(L)^{\text{SO}(3)}$, $0 \leq L \leq 6$ irreducible representations.

i	$\Gamma_{\text{final}}^{\text{SO}(3)}$	$g_i^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)} ; \Gamma_4^{\text{SO}(3)} ; \lambda \right)$
1	(0)	$\frac{1+\lambda^2+4\lambda^3+\lambda^4+\lambda^6}{(1-\lambda^2)^9}$
1	(1)	$\frac{4\lambda+6\lambda^2+4\lambda^3+6\lambda^4+4\lambda^5}{(1-\lambda^2)^9}$
1,2	(2)	$\frac{10\lambda^2+20\lambda^3+10\lambda^4}{(1-\lambda^2)^9}$
2	(3)	$\frac{20\lambda^3+28\lambda^4+8\lambda^5}{(1-\lambda^2)^9} + \frac{14\lambda^4+8\lambda^5}{(1-\lambda^2)^8} + \frac{3\lambda^4+4\lambda^5+\lambda^6}{(1-\lambda^2)^7}$
2	(4)	$\frac{35\lambda^4+36\lambda^5+\lambda^6}{(1-\lambda^2)^9} + \frac{36\lambda^5+19\lambda^6}{(1-\lambda^2)^8} + \frac{12\lambda^5+15\lambda^6+4\lambda^7}{(1-\lambda^2)^7}$
3	(5)	$\frac{44\lambda^5+44\lambda^6}{(1-\lambda^2)^9} + \frac{12\lambda^5+66\lambda^6+32\lambda^7}{(1-\lambda^2)^8} + \frac{30\lambda^6+36\lambda^7+10\lambda^8}{(1-\lambda^2)^7}$
3	(6)	$\frac{52\lambda^6+52\lambda^7}{(1-\lambda^2)^9} + \frac{32\lambda^6+104\lambda^7+46\lambda^8}{(1-\lambda^2)^8} + \frac{60\lambda^7+70\lambda^8+20\lambda^9}{(1-\lambda^2)^7}$
3	(7)	$\frac{60\lambda^7+60\lambda^8}{(1-\lambda^2)^9} + \frac{60\lambda^7+150\lambda^8+60\lambda^9}{(1-\lambda^2)^8} + \frac{105\lambda^8+120\lambda^9+35\lambda^{10}}{(1-\lambda^2)^7}$
3	\vdots	
3	(14)	$\frac{116\lambda^{14}+116\lambda^{15}}{(1-\lambda^2)^9} + \frac{564\lambda^{14}+696\lambda^{15}+74\lambda^{16}}{(1-\lambda^2)^8} + \frac{1092\lambda^{15}+1170\lambda^{16}+364\lambda^{17}}{(1-\lambda^2)^7}$
3	(15)	$\frac{124\lambda^{15}+124\lambda^{16}}{(1-\lambda^2)^9} + \frac{692\lambda^{15}+806\lambda^{16}+52\lambda^{17}}{(1-\lambda^2)^8} + \frac{1365\lambda^{16}+1456\lambda^{17}+455\lambda^{18}}{(1-\lambda^2)^7}$
3	(16)	$\frac{132\lambda^{16}+132\lambda^{17}}{(1-\lambda^2)^9} + \frac{837\lambda^{16}+924\lambda^{17}+21\lambda^{18}}{(1-\lambda^2)^8} + \frac{1680\lambda^{17}+1785\lambda^{18}+560\lambda^{19}}{(1-\lambda^2)^7}$
4	(17)	$\frac{140\lambda^{17}+140\lambda^{18}}{(1-\lambda^2)^9} + \frac{980\lambda^{17}+1050\lambda^{18}}{(1-\lambda^2)^8} + \frac{20\lambda^{17}+2040\lambda^{18}+2160\lambda^{19}+680\lambda^{20}}{(1-\lambda^2)^7}$
4	(18)	$\frac{148\lambda^{18}+148\lambda^{19}}{(1-\lambda^2)^9} + \frac{1110\lambda^{18}+1184\lambda^{19}}{(1-\lambda^2)^8} + \frac{72\lambda^{18}+2448\lambda^{19}+2584\lambda^{20}+816\lambda^{21}}{(1-\lambda^2)^7}$
4	(19)	$\frac{156\lambda^{19}+156\lambda^{20}}{(1-\lambda^2)^9} + \frac{1248\lambda^{19}+1326\lambda^{20}}{(1-\lambda^2)^8} + \frac{136\lambda^{19}+2907\lambda^{20}+3060\lambda^{21}+969\lambda^{22}}{(1-\lambda^2)^7}$
4	\vdots	

7. Generating function for five vectors

$$\begin{aligned}
 &g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)} ; \Gamma_5^{\text{SO}(3)} ; \lambda \right) \\
 &= \frac{\mathcal{N}_1 \left(\Gamma_{\text{final}}^{\text{SO}(3)} ; \Gamma_5^{\text{SO}(3)} ; \lambda \right)}{(1-\lambda^2)^{12}},
 \end{aligned} \tag{28}$$

$$\mathcal{N}_1 \left(\Gamma_{\text{final}}^{\text{SO}(3)} ; \Gamma_5^{\text{SO}(3)} ; \lambda \right)$$

$$\begin{aligned}
&= \frac{(L+4)(L+3)(L+2)(L+1)}{24}\lambda^L + \frac{(L+4)(L+3)(L+2)L}{6}\lambda^{L+1} \\
&+ \frac{(L+4)(L+3)(L+2)(L+1)}{8}\lambda^{L+2} - \frac{(L+4)(L+3)(L^2-3L-\frac{5}{2})}{3}\lambda^{L+3} \\
&- \frac{(L+4)(L+3)(L-3)(7L+2)}{12}\lambda^{L+4} - \frac{(L+4)(L-3)(2L+1)}{2}\lambda^{L+5} \\
&+ \frac{(L+4)(L-2)(L-3)(7L+5)}{12}\lambda^{L+6} + \frac{(L-2)(L-3)(L^2+5L+\frac{3}{2})}{3}\lambda^{L+7} \\
&- \frac{L(L-1)(L-2)(L-3)}{8}\lambda^{L+8} - \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+9} \\
&- \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+10} \\
&g_2^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
&= \frac{\mathcal{N}_{2,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{2,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{2,3}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{10}} \\
&+ \frac{\mathcal{N}_{2,4}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^9} \tag{29} \\
&\mathcal{N}_{2,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
&= \frac{(L+4)(L+3)(L+2)(L+1)}{24}\lambda^L + 20(2L+1)\lambda^{L+1} \\
&+ \left(-\frac{1}{24}L^4 - \frac{5}{12}L^3 - \frac{35}{24}L^2 + \frac{455}{12}L + 19\right)\lambda^{L+2} \\
&\mathcal{N}_{2,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
&= \left(\frac{1}{6}L^4 + \frac{3}{2}L^3 + \frac{13}{3}L^2 - 36L - 20\right)\lambda^{L+1} \\
&- \frac{(L-3)(L^3+13L^2-406L-208)}{24}\lambda^{L+2} \\
&- \frac{(L-3)(L^3+12L^2-58L-30)}{6}\lambda^{L+3} \\
&\mathcal{N}_{2,3}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
&= -\frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^{L+2} - \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+3} \\
&\mathcal{N}_{2,4}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
&= \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3} \\
&+ \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4} \\
&g_3^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)
\end{aligned}$$

$$\begin{aligned}
 &= \frac{\mathcal{N}_{3,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{3,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{3,3}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{10}} \\
 &\quad + \frac{\mathcal{N}_{3,4}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^9} \tag{30}
 \end{aligned}$$

$$\begin{aligned}
 &\mathcal{N}_{3,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= \frac{(L+4)(L+3)(L+2)(L+1)}{24} \lambda^L + 20(2L+1) \lambda^{L+1} \\
 &\quad + \left(-\frac{1}{24}L^4 - \frac{5}{12}L^3 - \frac{35}{24}L^2 + \frac{455}{12}L + 19\right) \lambda^{L+2} \\
 &\mathcal{N}_{3,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= 5(2L+1)(2L-7) \lambda^{L+1} - \frac{(L-3)(L^3 + 13L^2 - 406L - 208)}{24} \lambda^{L+2} \\
 &\mathcal{N}_{3,3}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= \frac{(L-3)(L^3 + 12L^2 - 58L - 30)}{6} \lambda^{L+1} \\
 &\quad - \frac{(L-2)(L-3)(L^2 - 81L - 40)}{24} \lambda^{L+2} \\
 &\quad - \frac{(L-2)(L-3)(L^2 - 10L - 6)}{6} \lambda^{L+3} \\
 &\mathcal{N}_{3,4}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= \frac{L(L-1)(L-2)(L-3)}{4} \lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6} \lambda^{L+3} \\
 &\quad + \frac{L(L-1)(L-2)(L-3)}{24} \lambda^{L+4} \\
 &g_4^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= \frac{\mathcal{N}_{4,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{4,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{4,3}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^{10}} \\
 &\quad + \frac{\mathcal{N}_{4,4}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right)}{(1-\lambda^2)^9} \tag{31} \\
 &\mathcal{N}_{4,1}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= 20(2L+1) \lambda^L + 20(2L+1) \lambda^{L+1} \\
 &\mathcal{N}_{4,2}^{\text{SO}(3)}\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda\right) \\
 &= \left(\frac{1}{24}L^4 + \frac{5}{12}L^3 + \frac{35}{24}L^2 - \frac{455}{12}L - 19\right) \lambda^L + 5(2L+1)(2L-7) \lambda^{L+1} \\
 &\quad - \frac{(L-3)(L^3 + 13L^2 - 406L - 208)}{24} \lambda^{L+2}
 \end{aligned}$$

$$\begin{aligned}
& \mathcal{N}_{4,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{(L-3)(L^3 + 12L^2 - 58L - 30)}{6} \lambda^{L+1} - \frac{(L-2)(L-3)(L^2 - 81L - 40)}{24} \lambda^{L+2} \\
&\quad - \frac{(L-2)(L-3)(L^2 - 10L - 6)}{6} \lambda^{L+3} \\
& \mathcal{N}_{4,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{L(L-1)(L-2)(L-3)}{4} \lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6} \lambda^{L+3} \\
&\quad + \frac{L(L-1)(L-2)(L-3)}{24} \lambda^{L+4} \\
& g_5^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{\mathcal{N}_{5,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{5,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{5,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{10}} \\
&\quad + \frac{\mathcal{N}_{5,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^9} \tag{32}
\end{aligned}$$

$$\begin{aligned}
& \mathcal{N}_{5,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 20(2L+1)\lambda^L + 20(2L+1)\lambda^{L+1} \\
& \mathcal{N}_{5,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \left(\frac{1}{24}L^4 + \frac{5}{12}L^3 + \frac{35}{24}L^2 - \frac{455}{12}L - 19 \right) \lambda^L + 5(2L+1)(2L-7)\lambda^{L+1} \\
&\quad - \frac{(L-3)(L^3 + 13L^2 - 406L - 208)}{24} \lambda^{L+2} \\
& \mathcal{N}_{5,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= (L-3)(2L-7)(2L+1)\lambda^{L+1} - \frac{(L-2)(L-3)(L^2 - 81L - 40)}{24} \lambda^{L+2} \\
& \mathcal{N}_{5,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{(L-2)(L-3)(L^2 - 10L - 6)}{6} \lambda^{L+1} + \frac{L(L-1)(L-2)(L-3)}{4} \lambda^{L+2} \\
&\quad + \frac{(L+1)(L-1)(L-2)(L-3)}{6} \lambda^{L+3} + \frac{L(L-1)(L-2)(L-3)}{24} \lambda^{L+4} \\
& g_6^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{\mathcal{N}_{6,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{6,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{6,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{10}} \\
&\quad + \frac{\mathcal{N}_{6,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^9} \tag{33}
\end{aligned}$$

$$\begin{aligned}
& \mathcal{N}_{6,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 20(2L+1)\lambda^L + 20(2L+1)\lambda^{L+1} \\
& \mathcal{N}_{6,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 5(2L+1)(2L-9)\lambda^L + 5(2L+1)(2L-7)\lambda^{L+1} \\
& \mathcal{N}_{6,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{(L-3)(L^3+13L^2-406L-208)}{24}\lambda^L + (L-3)(2L+1)(2L-7)\lambda^{L+1} \\
&\quad - \frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^{L+2} \\
& \mathcal{N}_{6,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+1} + \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2} \\
&\quad + \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3} + \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4} \\
& g_7^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{\mathcal{N}_{7,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{7,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{7,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{10}} \\
&\quad + \frac{\mathcal{N}_{7,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^9} \tag{34} \\
& \mathcal{N}_{7,1}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 20(2L+1)\lambda^L + 20(2L+1)\lambda^{L+1} \\
& \mathcal{N}_{7,2}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 5(2L+1)(2L-9)\lambda^L + 5(2L+1)(2L-7)\lambda^{L+1} \\
& \mathcal{N}_{7,3}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= 2(L-3)(L-6)(2L+1)\lambda^L + (L-3)(2L+1)(2L-7)\lambda^{L+1} \\
& \mathcal{N}_{7,4}^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^L + \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+1} \\
&\quad + \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3} \\
&\quad + \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4}
\end{aligned}$$

8. Conjectures

Let us sum up the expressions for two, three, four and five vectors:

8.1. Two vectors

$$g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_2^{\text{SO}(3)}; \lambda \right) = \frac{c_{2,1,L}\lambda^L + c_{2,1,L+1}\lambda^{L+1}}{(1-\lambda^2)^3}.$$

8.2. Three vectors

$$\begin{aligned} & g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_3^{\text{SO}(3)}; \lambda \right) \\ &= \frac{c_{3,1,L}\lambda^L + c_{3,1,L+1}\lambda^{L+1} + c_{3,1,L+3}\lambda^{L+3} + c_{3,1,L+4}\lambda^{L+4}}{(1-\lambda^2)^6}, \\ & g_2^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_3^{\text{SO}(3)}; \lambda \right) \\ &= \frac{c_{3,2^0,L}\lambda^L + c_{3,2^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^6} \\ & \quad + \frac{c_{3,2^1,L}\lambda^L + c_{3,2^1,L+1}\lambda^{L+1} + c_{3,2^1,L+2}\lambda^{L+2}}{(1-\lambda^2)^5}, \end{aligned}$$

8.3. Four vectors

$$\begin{aligned} & g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\ &= \frac{\mathcal{N} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^9}, \\ & \mathcal{N} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\ &= c_{4,1,L}\lambda^L + c_{4,1,L+1}\lambda^{L+1} + c_{4,1,L+2}\lambda^{L+2} + c_{4,1,L+3}\lambda^{L+3} \\ & \quad + c_{4,1,L+4}\lambda^{L+4} + c_{4,1,L+5}\lambda^{L+5} + c_{4,1,L+6}\lambda^{L+6} + c_{4,1,L+7}\lambda^{L+7} \\ & g_2^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\ &= \frac{c_{4,2^0,L}\lambda^L + c_{4,2^0,L+1}\lambda^{L+1} + c_{4,2^0,L+2}\lambda^{L+2}}{(1-\lambda^2)^9} \\ & \quad + \frac{c_{4,2^1,L+1}\lambda^{L+1} + c_{4,2^1,L+2}\lambda^{L+2}}{(1-\lambda^2)^8} \\ & \quad + \frac{c_{4,2^2,L+1}\lambda^{L+1} + c_{4,2^2,L+2}\lambda^{L+2} + c_{4,2^2,L+3}\lambda^{L+3}}{(1-\lambda^2)^7} \\ & g_3^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\ &= \frac{c_{4,3^0,L}\lambda^L + c_{4,3^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^9} \\ & \quad + \frac{c_{4,3^1,L}\lambda^L + c_{4,3^1,L+1}\lambda^{L+1} + c_{4,3^1,L+2}\lambda^{L+2}}{(1-\lambda^2)^8} \\ & \quad + \frac{c_{4,3^2,L+1}\lambda^{L+1} + c_{4,3^2,L+2}\lambda^{L+2} + c_{4,3^2,L+3}\lambda^{L+3}}{(1-\lambda^2)^7} \end{aligned}$$

$$\begin{aligned}
 & g_4^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_4^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{c_{4,4^0,L} \lambda^L + c_{4,4^0,L+1} \lambda^{L+1}}{(1-\lambda^2)^9} \\
 &+ \frac{c_{4,4^1,L} \lambda^L + c_{4,4^1,L+1} \lambda^{L+1}}{(1-\lambda^2)^8} \\
 &+ \frac{c_{4,4^2,L} \lambda^L + c_{4,4^2,L+1} \lambda^{L+1} + c_{4,4^2,L+2} \lambda^{L+2} + c_{4,4^2,L+3} \lambda^{L+3}}{(1-\lambda^2)^7}
 \end{aligned}$$

8.4. Five vectors

$$\begin{aligned}
 & g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{\mathcal{N}_1 \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)}{(1-\lambda^2)^{12}}, \\
 & \mathcal{N}_1 \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
 &= c_{5,1,L} \lambda^L + c_{5,1,L+1} \lambda^{L+1} + c_{5,1,L+2} \lambda^{L+2} + c_{5,1,L+3} \lambda^{L+3} \\
 &+ c_{5,1,L+4} \lambda^{L+4} + c_{5,1,L+5} \lambda^{L+5} + c_{5,1,L+6} \lambda^{L+6} + c_{5,1,L+7} \lambda^{L+7} \\
 &+ c_{5,1,L+8} \lambda^{L+8} + c_{5,1,L+9} \lambda^{L+9} + c_{5,1,L+10} \lambda^{L+10} \\
 & g_2^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{c_{5,2^0,L} \lambda^L + c_{5,2^0,L+1} \lambda^{L+1} + c_{5,2^0,L+2} \lambda^{L+2}}{(1-\lambda^2)^{12}} \\
 &+ \frac{c_{5,2^1,L+1} \lambda^{L+1} + c_{5,2^1,L+2} \lambda^{L+2} + c_{5,2^1,L+3} \lambda^{L+3}}{(1-\lambda^2)^{11}} \\
 &+ \frac{c_{5,2^2,L+2} \lambda^{L+2} + c_{5,2^2,L+3} \lambda^{L+3}}{(1-\lambda^2)^{10}} \\
 &+ \frac{c_{5,2^3,L+2} \lambda^{L+2} + c_{5,2^3,L+3} \lambda^{L+3} + c_{5,2^3,L+4} \lambda^{L+4}}{(1-\lambda^2)^9} \\
 & g_3^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
 &= \frac{c_{5,3^0,L} \lambda^L + c_{5,3^0,L+1} \lambda^{L+1} + c_{5,3^0,L+2} \lambda^{L+2}}{(1-\lambda^2)^{12}} \\
 &+ \frac{c_{5,3^1,L+1} \lambda^{L+1} + c_{5,3^1,L+2} \lambda^{L+2}}{(1-\lambda^2)^{11}} \\
 &+ \frac{c_{5,3^2,L+1} \lambda^{L+1} + c_{5,3^2,L+2} \lambda^{L+2} + c_{5,3^2,L+3} \lambda^{L+3}}{(1-\lambda^2)^{10}} \\
 &+ \frac{c_{5,3^3,L+2} \lambda^{L+2} + c_{5,3^3,L+3} \lambda^{L+3} + c_{5,3^3,L+4} \lambda^{L+4}}{(1-\lambda^2)^9} \\
 & g_4^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)
 \end{aligned}$$

$$\begin{aligned}
&= \frac{c_{5,4^0,L}\lambda^L + c_{5,4^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^{12}} \\
&+ \frac{c_{5,4^1,L}\lambda^L + c_{5,4^1,L+1}\lambda^{L+1} + c_{5,4^1,L+2}\lambda^{L+2}}{(1-\lambda^2)^{11}} \\
&+ \frac{c_{5,4^2,L+1}\lambda^{L+1} + c_{5,4^2,L+2}\lambda^{L+2} + c_{5,4^2,L+3}\lambda^{L+3}}{(1-\lambda^2)^{10}} \\
&+ \frac{c_{5,4^3,L+2}\lambda^{L+2} + c_{5,4^3,L+3}\lambda^{L+3} + c_{5,4^3,L+4}\lambda^{L+4}}{(1-\lambda^2)^9} \\
g_5^{\text{SO}(3)} &\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{c_{5,5^0,L}\lambda^L + c_{5,5^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^{12}} \\
&+ \frac{c_{5,5^1,L}\lambda^L + c_{5,5^1,L+1}\lambda^{L+1} + c_{5,5^1,L+2}\lambda^{L+2}}{(1-\lambda^2)^{11}} \\
&+ \frac{c_{5,5^2,L+1}\lambda^{L+1} + c_{5,5^2,L+2}\lambda^{L+2}}{(1-\lambda^2)^{10}} \\
&+ \frac{c_{5,5^3,L+1}\lambda^{L+1} + c_{5,5^3,L+2}\lambda^{L+2} + c_{5,5^3,L+3}\lambda^{L+3} + c_{5,5^3,L+4}\lambda^{L+4}}{(1-\lambda^2)^9} \\
g_6^{\text{SO}(3)} &\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{c_{5,6^0,L}\lambda^L + c_{5,6^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^{12}} \\
&+ \frac{c_{5,6^1,L}\lambda^L + c_{5,6^1,L+1}\lambda^{L+1}}{(1-\lambda^2)^{11}} \\
&+ \frac{c_{5,6^2,L}\lambda^L + c_{5,6^2,L+1}\lambda^{L+1} + c_{5,6^2,L+2}\lambda^{L+2}}{(1-\lambda^2)^{10}} \\
&+ \frac{c_{5,6^3,L+1}\lambda^{L+1} + c_{5,6^3,L+2}\lambda^{L+2} + c_{5,6^3,L+3}\lambda^{L+3} + c_{5,6^3,L+4}\lambda^{L+4}}{(1-\lambda^2)^9} \\
g_7^{\text{SO}(3)} &\left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right) \\
&= \frac{c_{5,7^0,L}\lambda^L + c_{5,7^0,L+1}\lambda^{L+1}}{(1-\lambda^2)^{12}} \\
&+ \frac{c_{5,7^1,L}\lambda^L + c_{5,7^1,L+1}\lambda^{L+1}}{(1-\lambda^2)^{11}} \\
&+ \frac{c_{5,7^2,L}\lambda^L + c_{5,7^2,L+1}\lambda^{L+1}}{(1-\lambda^2)^{10}} \\
&+ \frac{c_{5,7^3,L}\lambda^L + c_{5,7^3,L+1}\lambda^{L+1} + c_{5,7^3,L+2}\lambda^{L+2} + c_{5,7^3,L+3}\lambda^{L+3} + c_{5,7^3,L+4}\lambda^{L+4}}{(1-\lambda^2)^9}
\end{aligned}$$

8.5. Conjecture 1

We conjecture that for any N and any L (i.e. any $\Gamma_{\text{final}}^{\text{SO}(3)}$) the Molien function can be cast in the form of a sum of k (with $1 \leq k \leq 3N - 2$) rational fractions with all numerator polynomials having only non-negative coefficients:

$$g_h^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)} = (L); \Gamma_N^{\text{SO}(3)}; \lambda \right) = \sum_{l=1}^k \sum_{n \leq 0}^d \frac{c_{N,h^l,L+n} \lambda^{L+n}}{(1 - \lambda^2)^{3N-2-l}} \quad \text{with all } c_{N,h^l,L+n} \geq 0 \quad (35)$$

A simpler notation would be (there are several possible forms, but the index h is somewhat redundant with L , since the constraints $c_{N,h^l,L+n} \geq 0$ essentially fix the correct form. There are L -values where 2 different h are possible but the form is in fact the same.) :

$$g^{\text{SO}(3)} \left((L); \Gamma_N^{\text{SO}(3)}; \lambda \right) = \sum_{l=1}^k \sum_{n \leq 0}^d \frac{c_{N,L,l,n} \lambda^{L+n}}{(1 - \lambda^2)^{3N-2-l}} \quad \text{with all } c_{N,L,l,n} \geq 0 \quad (36)$$

Note that numerator λ -exponents start at L , since (L) -covariants are at least of total degree L . Such an expression admits the symbolic interpretation in terms of generalized integrity basis already proposed in our previous work on $\text{SO}(2)$ [1]. That is to say, if the least integer k for which such an expression holds is equal to 1, then the usual Molien function interpretation in terms of integrity basis holds. Else, if it is strictly more than 1, then necessarily $L > 0$, the module of (L) -covariants is non free but it is a sum of k submodules, each of these submodules, (if non zero,) is a free module that corresponds to the l^{th} rational fraction symbolic interpretation in terms of integrity basis ($1 \leq l \leq k$), so it is a module on a ring generated by $3N - 2 - l$ primary invariants and the minimal number of covariant generators of degree $L + n$ is given by $c_{N,L,l,n}$. So, this conjecture is in fact closely related to that of Stanley: conjecture 5.1 of Ref. [7]

In practice for a given pair (N, L) , expression Eq. (35) can be determined algorithmically by starting with the $g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)} = (L); \Gamma_N^{\text{SO}(3)}; \lambda \right)$ expression. If for the L -value considered, the numerator $\mathcal{N}_1 \left((L) = \Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_N^{\text{SO}(3)}; \lambda \right)$ has only non-negative coefficients, then one stops, otherwise we divide it by $1 - \lambda^2$. The division process itself is stopped not when the degree of the rest is less than 2 as one would do in usual Euclidian polynomial division, but when the rest's coefficients become non-negative for the L -value considered, which will happen according to the conjecture. It will constitute the numerator of the first fraction. If the so-obtained quotient has only non-negative coefficients for the L -value considered, one stops, otherwise the process is iterated, that is to say, the quotient is divided in the same way by $1 - \lambda^2$ and the new rest will constitute the numerator of the second fraction. And so on, until the quotient has also only non-negative

coefficients, which will happen according to the conjecture.

For example, for $N = 3$, the initial expression is suitable for $L < 2$. For $L \geq 2$, we obtain successively by the division process of the initial numerator:

$$\begin{aligned}
 & \frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} - (L+1)(L-1)\lambda^{L+3} - \frac{L(L-1)}{2}\lambda^{L+4} \\
 = & (1-\lambda^2) \left(\frac{L(L-1)}{2}\lambda^{L+2} \right) + \frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} - \frac{L(L-1)}{2}\lambda^{L+2} - (L+1)(L-1)\lambda^{L+3} \\
 = & (1-\lambda^2) \left((L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2} \right) + \frac{(L+2)(L+1)}{2}\lambda^L + (2L+1)\lambda^{L+1} - \frac{L(L-1)}{2}\lambda^{L+2} \\
 = & (1-\lambda^2) \left(\frac{L(L-1)}{2}\lambda^L + (L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2} \right) + (2L+1)\lambda^L + (2L+1)\lambda^{L+1}
 \end{aligned} \tag{37}$$

The “rest” $(2L+1)\lambda^L + (2L+1)\lambda^{L+1}$ having only non negative coefficients, is the numerator of the first fraction we are seeking for. The “quotient” $\frac{L(L-1)}{2}\lambda^L + (L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}$ happens in this simple case to have only non negative coefficients for $L \geq 2$. So there will be only two fractions and it will constitute the numerator of the second fraction.

For $N = 4$, the initial expression is suitable for $L < 3$. For $L \geq 3$, we obtain successively by the division process of the initial numerator:

$$\begin{aligned}
 & \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} + \frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2} - \frac{(L+3)(L-2)(5L+4)}{6}\lambda^{L+3} \\
 & - \frac{(L+3)(L-2)(5L+1)}{6}\lambda^{L+4} + \frac{L(L-1)(L-2)}{6}\lambda^{L+5} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+6} + \frac{L(L-1)(L-2)}{6}\lambda^{L+7} \\
 = & (1-\lambda^2) \left(-\frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} + \frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2} \\
 & - \frac{(L+3)(L-2)(5L+4)}{6}\lambda^{L+3} - \frac{(L+3)(L-2)(5L+1)}{6}\lambda^{L+4} + \frac{L(L-1)(L-2)}{3}\lambda^{L+5} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+6} \\
 = & (1-\lambda^2) \left(-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4} - \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} \\
 & + \frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2} - \frac{(L+3)(L-2)(5L+4)}{6}\lambda^{L+3} - \frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+4} + \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \\
 = & (1-\lambda^2) \left(-\frac{L(L-1)(L-2)}{3}\lambda^{L+3} - \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4} - \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L \\
 & + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} + \frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2} - \frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3} - \frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+4} \\
 = & (1-\lambda^2) \left(\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2} - \frac{L(L-1)(L-2)}{3}\lambda^{L+3} - \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4} - \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) \\
 & + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} - \frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2} - \frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3} \\
 = & (1-\lambda^2) \left(\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2} - \frac{L(L-1)(L-2)}{3}\lambda^{L+3} - \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4} - \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) \\
 & + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1} - \frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2} - \frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3} \\
 = & (1-\lambda^2) \left(\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1} + \frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2} - \frac{L(L-1)(L-2)}{3}\lambda^{L+3} - \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4} \right. \\
 & \left. - \frac{L(L-1)(L-2)}{6}\lambda^{L+5} \right) + \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + 4(2L+1)\lambda^{L+1} - \frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2}
 \end{aligned} \tag{38}$$

$$\begin{aligned}
 &= (1 - \lambda^2) \left(\frac{(L^3 + 6L^2 - 37L - 18)}{6} \lambda^L + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} + \frac{(L - 2)(L^2 + 8L + 3)}{3} \lambda^{L+2} - \frac{L(L - 1)(L - 2)}{3} \lambda^{L+3} \right. \\
 &\quad \left. - \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+4} - \frac{L(L - 1)(L - 2)}{6} \lambda^{L+5} \right) + 4(2L + 1)\lambda^L + 4(2L + 1)\lambda^{L+1} \quad (39)
 \end{aligned}$$

For $L = 3$ and $L = 4$ one must stop at Eq. (39), where all coefficients of the rest are positive, whereas for larger values of L the coefficient of λ^{L+2} is negative in the rest of Eq. (39) and one must stop only at Eq. (39). Let us consider first the cases $L = 3$ and $L = 4$. The quotient has negative coefficients and must be divided again by $(1 - \lambda^2)$,

$$\begin{aligned}
 &\frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} + \frac{(L - 2)(L^2 + 8L + 3)}{3} \lambda^{L+2} - \frac{L(L - 1)(L - 2)}{3} \lambda^{L+3} - \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+4} - \frac{L(L - 1)(L - 2)}{6} \lambda^{L+5} \\
 &= (1 - \lambda^2) \left(\frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} + \frac{(L - 2)(L^2 + 8L + 3)}{3} \lambda^{L+2} - \frac{L(L - 1)(L - 2)}{2} \lambda^{L+3} \\
 &\quad - \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+4} \\
 &= (1 - \lambda^2) \left(\frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+2} + \frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} - \frac{(L - 2)(L^2 - 16L - 9)}{6} \lambda^{L+2} \\
 &\quad - \frac{L(L - 1)(L - 2)}{2} \lambda^{L+3} \\
 &= (1 - \lambda^2) \left(\frac{L(L - 1)(L - 2)}{2} \lambda^{L+1} + \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+2} + \frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + 2(L - 2)(2L + 1)\lambda^{L+1} \\
 &\quad - \frac{(L - 2)(L^2 - 16L - 9)}{6} \lambda^{L+2} \quad (40)
 \end{aligned}$$

This time both rest and quotient have non negative coefficients, so we stop here and retrieve the numerators of the second and third fractions of $g_2^{\text{SO}(3)}$ in Eq. (25). For $L > 4$, we have to divide the quotient of Eq. (39) by $(1 - \lambda^2)$,

$$\begin{aligned}
 &\frac{(L^3 + 6L^2 - 37L - 18)}{6} \lambda^L + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} + \frac{(L - 2)(L^2 + 8L + 3)}{3} \lambda^{L+2} - \frac{L(L - 1)(L - 2)}{3} \lambda^{L+3} \\
 &\quad - \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+4} - \frac{L(L - 1)(L - 2)}{6} \lambda^{L+5} \\
 &= (1 - \lambda^2) \left(\frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + \frac{(L^3 + 6L^2 - 37L - 18)}{6} \lambda^L + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} + \frac{(L - 2)(L^2 + 8L + 3)}{3} \lambda^{L+2} \\
 &\quad - \frac{L(L - 1)(L - 2)}{2} \lambda^{L+3} - \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+4} \\
 &= (1 - \lambda^2) \left(\frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+2} + \frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + \frac{(L^3 + 6L^2 - 37L - 18)}{6} \lambda^L + \frac{(L - 2)(L^2 + 7L + 4)}{2} \lambda^{L+1} \\
 &\quad - \frac{(L - 2)(L^2 - 16L - 9)}{6} \lambda^{L+2} - \frac{L(L - 1)(L - 2)}{2} \lambda^{L+3} \\
 &= (1 - \lambda^2) \left(\frac{L(L - 1)(L - 2)}{2} \lambda^{L+1} + \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+2} + \frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) + \frac{(L^3 + 6L^2 - 37L - 18)}{6} \lambda^L \\
 &\quad + 2(L - 2)(2L + 1)\lambda^{L+1} - \frac{(L - 2)(L^2 - 16L - 9)}{6} \lambda^{L+2} \quad (41) \\
 &= (1 - \lambda^2) \left(\frac{(L - 2)(L^2 - 16L - 9)}{6} \lambda^L + \frac{L(L - 1)(L - 2)}{2} \lambda^{L+1} + \frac{(L + 1)(L - 1)(L - 2)}{2} \lambda^{L+2} + \frac{L(L - 1)(L - 2)}{6} \lambda^{L+3} \right) \\
 &\quad + 2(L - 3)(2L + 1)\lambda^L + 2(L - 2)(2L + 1)\lambda^{L+1} \quad (42)
 \end{aligned}$$

For $5 \leq L \leq 16$ one must stop at Eq. (41), where all coefficients of the rest are positive, whereas for larger values of L the coefficient of λ^{L+2} is negative in the rest of Eq. (41) and one must stop only at Eq. (42). In both cases, the quotient has only non-negative

coefficients, so the rests and quotients of Eqs. (41) and (42) gives the numerators of the second and third fractions of $g_3^{\text{SO}(3)}$ and $g_4^{\text{SO}(3)}$ in Eqs. (26) and (27).

We leave it to the reader to treat the case $N = 5$.

8.6. Conjecture 2

For the electric dipole moment, the relevant covariant module which corresponds to the $(L)=(1)$ irreducible representation, will always be free. This conjecture is based on the observation that for a given N , $g_1^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)} = (L); \Gamma_N^{\text{SO}(3)}; \lambda \right)$ has the form of Eq. (35) for all L if $N = 1$ or $N = 2$ and for all $L < N$ if $5 \geq N > 2$.

9. Asymptotic expression of the generating function

See table 5.

9.1. Number of terms in the numerators of the asymptotic expression of the generating function

See table 6.

10. Finite groups

If in addition to the $\text{SO}(3)$ action there is a finite group action on the vector variables, it can be taken advantage of in a second step as was argued in [8] for the particular case of invariants. For example, for $N = 2$ which can be related as we have seen to the case of a triatomic molecule ABC, if the origin of the two vectors is A and if $B=C$, then the action of the permutation group \mathcal{S}_2 on the vectors $\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$ and $\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$ can be exploited to simplify the expression of the physical observables such as the DMS functions. In this particular case, we deduce for example that the polynomials of Eq. (20) must satisfy, $P_{z_1}[Q_1, Q_2, Q_3] = P_{z_2}[Q_2, Q_1, Q_3]$, and $P_{x_1 y_2 - y_1 x_2}[Q_1, Q_2, Q_3] = -P_{x_1 y_2 - y_1 x_2}[Q_2, Q_1, Q_3]$.

10.1. Introduction

The coordinates x, y, z of a spatial vector span a three-dimensional representation Γ_1 . We consider the representation Γ_n generated by n spatial vectors:

$$\Gamma_n = \Gamma_1 \oplus \cdots \oplus \Gamma_1.$$

10.1.1. Group C_i

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$D(i) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

10.1.2. Group T_d See table 8.

11. Conclusion

This is the conclusion.

Acknowledgments

Financial support for the project *Application de la Théorie des Invariants à la Physique Moléculaire* via a CNRS grant *Projet Exploratoire Premier Soutien (PEPS) Physique Théorique et Interfaces (PTI)* is acknowledged.

B. Z. thanks the Isaac Newton Institute for Mathematical Sciences for financial support making possible his visit within the program “Mathematics for liquid crystals” and for fruitful discussions during this visit.

Appendix A. Generating functions obtained by coupling

The Molien function with a reducible initial representation $g^G(\Gamma_{\text{final}}; \Gamma_{\text{initial},1} \oplus \Gamma_{\text{initial},2}; \lambda)$ can be calculated using Molien functions for the $\Gamma_{\text{initial},1}$ and $\Gamma_{\text{initial},2}$ initial representations, see Eq.(43) of [9]:

$$g^G(\Gamma_f; \Gamma_{i,1} \oplus \Gamma_{i,2}; \lambda) = \sum_{\Gamma_{f,1}} \sum_{\Gamma_{f,2}} n_{\Gamma_{f,1}, \Gamma_{f,2}}^{\Gamma_f} g^G(\Gamma_{f,1}; \Gamma_{i,1}; \lambda) g^G(\Gamma_{f,2}; \Gamma_{i,2}; \lambda), \text{ (A.1)}$$

where the symbol $n_{\Gamma_{f,1}, \Gamma_{f,2}}^{\Gamma_f}$ counts the irreducible representation of Γ_f in the product $\Gamma_{f,1} \otimes \Gamma_{f,2}$.

This paper deals with the group $G = \text{SO}(3)$. The initial representation $\Gamma_N^{\text{SO}(3)}$ originating from N spatial vectors is reducible:

$$\Gamma_N^{\text{SO}(3)} = \Gamma_1^{\text{SO}(3)} \oplus \Gamma_{N-1}^{\text{SO}(3)},$$

and The Molien function $g^{\text{SO}(3)}(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_N^{\text{SO}(3)}; \lambda)$ can be calculated using Eq. (A.1) with initial representations $\Gamma_{i,1} = \Gamma_1^{\text{SO}(3)}$ and $\Gamma_{i,2} = \Gamma_{N-1}^{\text{SO}(3)}$.

$$\begin{aligned}
 & g^{\text{SO}(3)} \left((L)^{\text{SO}(3)} ; \Gamma_N^{\text{SO}(3)} ; \lambda \right) \\
 &= \sum_{L_A=0}^{\infty} \sum_{L_B=0}^{\infty} n_{L_A, L_B}^L g^{\text{SO}(3)} \left((L_A)^{\text{SO}(3)} ; \Gamma_1^{\text{SO}(3)} ; \lambda \right) g^{\text{SO}(3)} \left((L_B)^{\text{SO}(3)} ; \Gamma_{N-1}^{\text{SO}(3)} ; \lambda \right) \quad (\text{A.2})
 \end{aligned}$$

$$\begin{aligned}
 & g^{\text{SO}(3)} \left((L)^{\text{SO}(3)} ; \Gamma_N^{\text{SO}(3)} ; \lambda \right) \\
 &= \sum_{L_A=0}^{\infty} \sum_{L_B=|L-L_A|}^{L_A+L} g^{\text{SO}(3)} \left((L_A)^{\text{SO}(3)} ; \Gamma_1^{\text{SO}(3)} ; \lambda \right) g^{\text{SO}(3)} \left((L_B)^{\text{SO}(3)} ; \Gamma_{N-1}^{\text{SO}(3)} ; \lambda \right) \\
 &= \sum_{L_A=0}^{L-1} \sum_{L_B=L-L_A}^{L_A+L} g^{\text{SO}(3)} \left((L_A)^{\text{SO}(3)} ; \Gamma_1^{\text{SO}(3)} ; \lambda \right) g^{\text{SO}(3)} \left((L_B)^{\text{SO}(3)} ; \Gamma_{N-1}^{\text{SO}(3)} ; \lambda \right) \\
 &\quad + \sum_{L_A=L}^{\infty} \sum_{L_B=L_A-L}^{L_A+L} g^{\text{SO}(3)} \left((L_A)^{\text{SO}(3)} ; \Gamma_1^{\text{SO}(3)} ; \lambda \right) g^{\text{SO}(3)} \left((L_B)^{\text{SO}(3)} ; \Gamma_{N-1}^{\text{SO}(3)} ; \lambda \right)
 \end{aligned}$$

We can check for concrete values of N that

$$\sum_{L=0}^{\infty} (2L+1) g^{\text{SO}(3)} \left((L)^{\text{SO}(3)} ; \Gamma_N^{\text{SO}(3)} ; \lambda \right) = \frac{1}{(1-\lambda)^{3N}}.$$

References

- [1] G. Dhont and B. I. Zhilinskiĭ. The action of the orthogonal group on planar vectors: invariants, covariants and syzygies. *J. Phys. A: Math. Theor.*, 46(45):455202 (27 pages), 2013.
- [2] T. Molien. Über die Invarianten der linearen substitutionsgruppen. *Sitzungsber. Königl. Preuss. Akad. Wiss.*, 52:1152–1156, 1897.
- [3] I. S. Gradshteyn and I. M. Ryzhik. Table of integrals, series, and products, 1980. Equation (3.616.7).
- [4] M. A. Collins and D. F. Parsons. Implications of rotation–inversion–permutation invariance for analytic molecular potential energy surfaces. *J. Chem. Phys.*, 99(9):6756–6772, 1993.
- [5] M. A. Morrison and G. A. Parker. A guide to rotations in quantum mechanics. *Aust. J. Phys.*, 40:465–497, 1987.
- [6] H. Weyl. *The Classical Groups. Their Invariants and Representations*. Princeton University Press, Princeton, New Jersey, 1939.
- [7] R. P. Stanley. Linear diophantine equations and local cohomology. *Invent. math.*, 68:175–193, 1982.
- [8] P. Cassam-Chenaï and F. Patras. Symmetry–adapted polynomial basis for global potential energy surfaces-applications to XY_4 molecules. *J. Math. Chem.*, 44:938–966, 2008.
- [9] L. Michel and B. I. Zhilinskiĭ. Symmetry, invariants, topology. Basic tools. *Phys. Rep.*, 341(1–6):11–84, 2001.

Table 4. Expressions of the $g_i^{\text{SO}(3)}$ Molien functions for five spatial vectors and the final $(L)^{\text{SO}(3)}$, $0 \leq L \leq 6$ irreducible representations.

i	$\Gamma_{\text{final}}^{\text{SO}(3)}$	$g_i^{\text{SO}(3)} \left(\Gamma_{\text{final}}^{\text{SO}(3)}; \Gamma_5^{\text{SO}(3)}; \lambda \right)$
1	(0)	$\frac{1+3\lambda^2+10\lambda^3+6\lambda^4+6\lambda^5+10\lambda^6+3\lambda^7+\lambda^9}{(1-\lambda^2)^{12}}$
1	(1)	$\frac{5\lambda+10\lambda^2+15\lambda^3+30\lambda^4+30\lambda^5+15\lambda^6+10\lambda^7+5\lambda^8}{(1-\lambda^2)^{12}}$
1	(2)	$\frac{15\lambda^2+40\lambda^3+45\lambda^4+45\lambda^5+40\lambda^6+15\lambda^7}{(1-\lambda^2)^{12}}$
1	(3)	$\frac{35\lambda^3+105\lambda^4+105\lambda^5+35\lambda^6}{(1-\lambda^2)^{12}}$
2	(4)	$\frac{70\lambda^4+180\lambda^5+110\lambda^6}{(1-\lambda^2)^{12}} + \frac{44\lambda^5+65\lambda^6+\lambda^7}{(1-\lambda^2)^{11}} + \frac{29\lambda^6+10\lambda^7}{(1-\lambda^2)^{10}} + \frac{6\lambda^6+5\lambda^7+\lambda^8}{(1-\lambda^2)^9}$
3	(5)	$\frac{126\lambda^5+220\lambda^6+94\lambda^7}{(1-\lambda^2)^{12}} + \frac{165\lambda^6+149\lambda^7}{(1-\lambda^2)^{11}} + \frac{35\lambda^6+105\lambda^7+31\lambda^8}{(1-\lambda^2)^{10}} + \frac{30\lambda^7+24\lambda^8+5\lambda^9}{(1-\lambda^2)^9}$
3	(6)	$\frac{210\lambda^6+260\lambda^7+50\lambda^8}{(1-\lambda^2)^{12}} + \frac{325\lambda^7+245\lambda^8}{(1-\lambda^2)^{11}} + \frac{135\lambda^7+245\lambda^8+60\lambda^9}{(1-\lambda^2)^{10}} + \frac{90\lambda^8+70\lambda^9+15\lambda^{10}}{(1-\lambda^2)^9}$
4	(7)	$\frac{300\lambda^7+300\lambda^8}{(1-\lambda^2)^{12}} + \frac{30\lambda^7+525\lambda^8+345\lambda^9}{(1-\lambda^2)^{11}} + \frac{330\lambda^8+465\lambda^9+90\lambda^{10}}{(1-\lambda^2)^{10}} + \frac{210\lambda^9+160\lambda^{10}+35\lambda^{11}}{(1-\lambda^2)^9}$
4	(8)	$\frac{340\lambda^8+340\lambda^9}{(1-\lambda^2)^{12}} + \frac{155\lambda^8+765\lambda^9+440\lambda^{10}}{(1-\lambda^2)^{11}} + \frac{655\lambda^9+780\lambda^{10}+110\lambda^{11}}{(1-\lambda^2)^{10}} + \frac{420\lambda^{10}+315\lambda^{11}+70\lambda^{12}}{(1-\lambda^2)^9}$
4	(9)	$\frac{380\lambda^9+380\lambda^{10}}{(1-\lambda^2)^{12}} + \frac{335\lambda^9+1045\lambda^{10}+520\lambda^{11}}{(1-\lambda^2)^{11}} + \frac{1149\lambda^{10}+1204\lambda^{11}+105\lambda^{12}}{(1-\lambda^2)^{10}} + \frac{756\lambda^{11}+560\lambda^{12}+126\lambda^{13}}{(1-\lambda^2)^9}$
4	(10)	$\frac{420\lambda^{10}+420\lambda^{11}}{(1-\lambda^2)^{12}} + \frac{581\lambda^{10}+1365\lambda^{11}+574\lambda^{12}}{(1-\lambda^2)^{11}} + \frac{1855\lambda^{11}+1750\lambda^{12}+56\lambda^{13}}{(1-\lambda^2)^{10}} + \frac{1260\lambda^{12}+924\lambda^{13}+210\lambda^{14}}{(1-\lambda^2)^9}$
5	(11)	$\frac{460\lambda^{11}+460\lambda^{12}}{(1-\lambda^2)^{12}} + \frac{905\lambda^{11}+1725\lambda^{12}+590\lambda^{13}}{(1-\lambda^2)^{11}} + \frac{2760\lambda^{12}+2430\lambda^{13}}{(1-\lambda^2)^{10}} + \frac{60\lambda^{12}+1980\lambda^{13}+1440\lambda^{14}+330\lambda^{15}}{(1-\lambda^2)^9}$
5	(12)	$\frac{500\lambda^{12}+500\lambda^{13}}{(1-\lambda^2)^{12}} + \frac{1320\lambda^{12}+2125\lambda^{13}+555\lambda^{14}}{(1-\lambda^2)^{11}} + \frac{3825\lambda^{13}+3255\lambda^{14}}{(1-\lambda^2)^{10}} + \frac{270\lambda^{13}+2970\lambda^{14}+2145\lambda^{15}+495\lambda^{16}}{(1-\lambda^2)^9}$
5	(13)	$\frac{540\lambda^{13}+540\lambda^{14}}{(1-\lambda^2)^{12}} + \frac{1840\lambda^{13}+2565\lambda^{14}+455\lambda^{15}}{(1-\lambda^2)^{11}} + \frac{5130\lambda^{14}+4235\lambda^{15}}{(1-\lambda^2)^{10}} + \frac{605\lambda^{14}+4290\lambda^{15}+3080\lambda^{16}+715\lambda^{17}}{(1-\lambda^2)^9}$
5	(14)	$\frac{580\lambda^{14}+580\lambda^{15}}{(1-\lambda^2)^{12}} + \frac{2480\lambda^{14}+3045\lambda^{15}+275\lambda^{16}}{(1-\lambda^2)^{11}} + \frac{6699\lambda^{15}+5379\lambda^{16}}{(1-\lambda^2)^{10}} + \frac{1100\lambda^{15}+6006\lambda^{16}+4290\lambda^{17}+1001\lambda^{18}}{(1-\lambda^2)^9}$
6	(15)	$\frac{620\lambda^{15}+620\lambda^{16}}{(1-\lambda^2)^{12}} + \frac{3255\lambda^{15}+3565\lambda^{16}}{(1-\lambda^2)^{11}} + \frac{\lambda^{15}+8556\lambda^{16}+6695\lambda^{17}}{(1-\lambda^2)^{10}} + \frac{1794\lambda^{16}+8190\lambda^{17}+5824\lambda^{18}+1365\lambda^{19}}{(1-\lambda^2)^9}$
6	(16)	$\frac{660\lambda^{16}+660\lambda^{17}}{(1-\lambda^2)^{12}} + \frac{3795\lambda^{16}+4125\lambda^{17}}{(1-\lambda^2)^{11}} + \frac{390\lambda^{16}+10725\lambda^{17}+8190\lambda^{18}}{(1-\lambda^2)^{10}} + \frac{2730\lambda^{17}+10920\lambda^{18}+7735\lambda^{19}+1820\lambda^{20}}{(1-\lambda^2)^9}$
6	(17)	$\frac{700\lambda^{17}+700\lambda^{18}}{(1-\lambda^2)^{12}} + \frac{4375\lambda^{17}+4725\lambda^{18}}{(1-\lambda^2)^{11}} + \frac{910\lambda^{17}+13230\lambda^{18}+9870\lambda^{19}}{(1-\lambda^2)^{10}} + \frac{3955\lambda^{18}+14280\lambda^{19}+10080\lambda^{20}+2380\lambda^{21}}{(1-\lambda^2)^9}$
6	:	:
6	(79)	$\frac{3180\lambda^{79}+3180\lambda^{80}}{(1-\lambda^2)^{12}} + \frac{118455\lambda^{79}+120045\lambda^{80}}{(1-\lambda^2)^{11}} + \frac{1715985\lambda^{79}+1824684\lambda^{80}+48279\lambda^{81}}{(1-\lambda^2)^{10}} + \frac{5310690\lambda^{80}+9015006\lambda^{81}+6086080\lambda^{82}+1502501\lambda^{83}}{(1-\lambda^2)^9}$
6	(80)	$\frac{3220\lambda^{80}+3220\lambda^{81}}{(1-\lambda^2)^{12}} + \frac{121555\lambda^{80}+123165\lambda^{81}}{(1-\lambda^2)^{11}} + \frac{1804726\lambda^{80}+1896741\lambda^{81}+30030\lambda^{82}}{(1-\lambda^2)^{10}} + \frac{5599594\lambda^{81}+9489480\lambda^{82}+6405399\lambda^{83}+1581580\lambda^{84}}{(1-\lambda^2)^9}$
6	(81)	$\frac{3260\lambda^{81}+3260\lambda^{82}}{(1-\lambda^2)^{12}} + \frac{124695\lambda^{81}+126325\lambda^{82}}{(1-\lambda^2)^{11}} + \frac{1896830\lambda^{81}+1970670\lambda^{82}+10270\lambda^{83}}{(1-\lambda^2)^{10}} + \frac{5900115\lambda^{82}+9982440\lambda^{83}+6737120\lambda^{84}+1663740\lambda^{85}}{(1-\lambda^2)^9}$
7	(82)	$\frac{3300\lambda^{82}+3300\lambda^{83}}{(1-\lambda^2)^{12}} + \frac{127875\lambda^{82}+129525\lambda^{83}}{(1-\lambda^2)^{11}} + \frac{1981320\lambda^{82}+2046495\lambda^{83}}{(1-\lambda^2)^{10}} + \frac{11060\lambda^{82}+6212560\lambda^{83}+10494360\lambda^{84}+7081560\lambda^{85}+1749060\lambda^{86}}{(1-\lambda^2)^9}$
7	(83)	$\frac{3340\lambda^{83}+3340\lambda^{84}}{(1-\lambda^2)^{12}} + \frac{131095\lambda^{83}+132765\lambda^{84}}{(1-\lambda^2)^{11}} + \frac{2057440\lambda^{83}+2124240\lambda^{84}}{(1-\lambda^2)^{10}} + \frac{34020\lambda^{83}+6537240\lambda^{84}+11025720\lambda^{85}+7439040\lambda^{86}+1837620\lambda^{87}}{(1-\lambda^2)^9}$
7	(84)	$\frac{3380\lambda^{84}+3380\lambda^{85}}{(1-\lambda^2)^{12}} + \frac{134355\lambda^{84}+136045\lambda^{85}}{(1-\lambda^2)^{11}} + \frac{2135484\lambda^{84}+2203929\lambda^{85}}{(1-\lambda^2)^{10}} + \frac{58671\lambda^{84}+6874470\lambda^{85}+11577006\lambda^{86}+7809885\lambda^{87}+1929501\lambda^{88}}{(1-\lambda^2)^9}$
7	:	:

Table 5. Values of L such that the asymptotic expression may be used to define an integrity basis.

n	$L_{\text{threshold}}$
3	1, 2, 3, ...
4	17, 18, 19, ...
5	82, 83, 84, ...
6	295, 296, 297, ...

Table 6. Number of terms in the numerators of the asymptotic expression of the generating function. The denominators are $(1 - \lambda^2)^n$.

n	numerator	
6	$(2L + 1)\lambda^L + (2L + 1)\lambda^{L+1}$	$2(2L + 1)$
5	$\frac{L(L-1)}{2}\lambda^L + (L + 1)(L - 1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}$	$(L - 1)(2L + 1)$
total		$(L + 1)(2L + 1)$
9	$4(2L + 1)\lambda^L + 4(2L + 1)\lambda^{L+1}$	$8(2L + 1)$
8	$2(L - 3)(2L + 1)\lambda^L + 2(L - 2)(2L + 1)\lambda^{L+1}$	$2(2L - 5)(2L + 1)$
7	$\frac{(L-2)(L^2-16L-9)}{6}\lambda^L + \frac{L(L-1)(L-2)}{2}\lambda^{L+1}$ $+ \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}$	$\frac{2}{3}(L - 3)(L - 2)(2L + 1)$
total		$\frac{2}{3}(L^2 + L + 3)(2L + 1)$
12	$20(2L + 1)\lambda^L + 20(2L + 1)\lambda^{L+1}$	$40(2L + 1)$
11	$5(2L + 1)(2L - 9)\lambda^L + 5(2L + 1)(2L - 7)\lambda^{L+1}$	$20(L - 4)(2L + 1)$
10	$2(L - 3)(L - 6)(2L + 1)\lambda^L$ $+ (L - 3)(2L + 1)(2L - 7)\lambda^{L+1}$	$(4L - 19)(L - 3)(2L + 1)$
9	$\frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^L + \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+1}$ $+ \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3}$ $+ \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4}$	$\frac{1}{6}(L - 3)(L - 2)(2L - 17)(2L + 1)$
total		$\frac{1}{6}L(2L^2 - 3L + 31)(2L + 1)$

Table 7. Generating functions $g^{C_i}(\Gamma_{\text{final}}; \Gamma_{\text{initial}}; \lambda)$

Γ_{initial}	Γ_{final}	$g^{C_i}(\Gamma_{\text{final}}; \Gamma_{\text{initial}}; \lambda)$
Γ_1	A_1	$\frac{1+3\lambda^2}{(1-\lambda^2)^3}$
Γ_1	A_2	$\frac{3\lambda+\lambda^3}{(1-\lambda^2)^3}$

Table 8. Number of terms in the numerator of the generating function for the invariants.

irrep	Γ_1	Γ_2	Γ_3	Γ_n
A_1	1	$ G $	$ G ^2$	$ G ^n$
A_2	1	$ G $	$ G ^2$	$ G ^n$
E	2	$2 G $	$2 G ^2$	$2 G ^n$
F_1	3	$3 G $	$3 G ^2$	$3 G ^n$
F_2	3	$3 G $	$3 G ^2$	$3 G ^n$