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Abstract. The present paper on invariant or covariant polynomials built from a set of three dimensional vectors under the action of the SO(3) group is a follow–up to our previous article [G. Dhont and B. I. Zhilinskií. The action of the orthogonal group on planar vectors: invariants, covariants and syzygies. J. Phys. A: Math. Theor., 46(45):455202 (27 pages), 2013.] dealing with a set of two dimensional vectors under the action of the SO(2) group.

The goal is to show how to obtain Molien functions for SO(3) invariant and covariant modules, how to recast them in an appropriate form when these modules are not free, and how to use them to build integrity bases for free modules or their generalization in the case of non-free covariants modules.

We also explain how to easily derive O(3) invariants and covariants basis from SO(3) ones . However, applications of SO(3) invariant and covariant bases extends to cases such as the modelling of potential energy or dipole moment hypersurfaces in quantum chemistry, where O(3)-symmetry is expected to hold, unless parity violation is considered, but where the use of the SO(3) invariant ring is more practical than that of O(3).

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1. Introduction

The present work on the SO(3) invariants and covariants built from N vectors of the three–dimensional space stems from two previous articles. The first one [1] dealing with planar vectors and SO(2) symmetry, which put forward the problem of dealing with non-free covariant modules that arise when dealing with non finite groups.

Our 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 the generating families.

The article is organized as follows: In the next section the Molien functions for up to 5 spatial vectors 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 explained in Appendix A considers the Molien function for only one spatial vector as the elementary building material from which are worked out the other Molien functions. In the third section, we use these explicit Molien functions to make two conjectures of practical importance to derive and employ families of generating functions in the perspective of fitting symmetry-adapted quantum mechanical quantities. In the last section, we explain a general method to actually build such generating families and apply it to the non trivial case of 3 spatial vectors. We provide results for both $SO(3)$ and $0(3)$ groups. However, we argue that despite the fact that molecular systems can be considered as invariant under spatial inversion, it is usually more useful to fit molecular potential energy and dipole moment hypersurfaces with $SO(3)$-covariant generating families. We conclude with our perspectives for this work.

2. Construction of the generating function for N vectors

2.1. Molien general integral formula

2.1.1. Rotation 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.

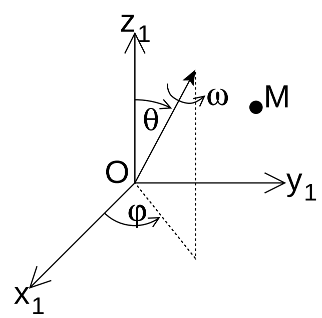

Figure 1. Parametrization of a rotation in three–dimensional space. The θ and φ angles are the spherical angles of the rotation axis, the ω angle is the rotation angle around the rotation axis.

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:

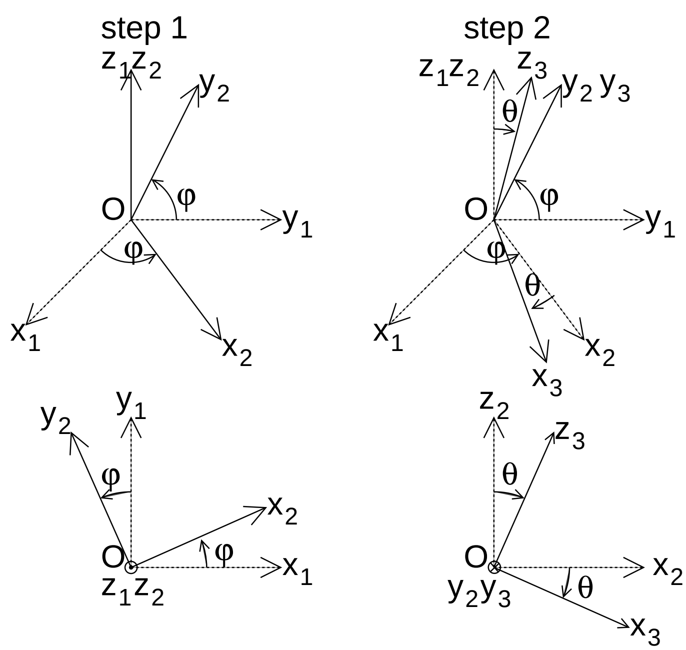

Figure 2. Definition of the $(Ox_3y_3z_3)$ frame.

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

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

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

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

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:

$$\begin{aligned} \begin{pmatrix} \vec{e}_{x_3} & \vec{e}_{y_3} & \vec{e}_{z_3} \end{pmatrix} &= \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \\ &= \begin{pmatrix} \vec{e}_{x_1} & \vec{e}_{y_1} & \vec{e}_{z_1} \end{pmatrix} \underbrace{\begin{pmatrix} \cos\varphi\cos\theta & -\sin\varphi & \cos\varphi\sin\theta \\ \sin\varphi\cos\theta & \cos\varphi & \sin\varphi\sin\theta \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}}_{=M_1(\theta,\varphi)}. \end{aligned} \qquad (3)$$

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:

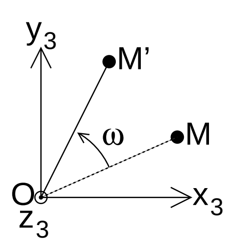

Figure 3. Rotation of point M in the $(Ox_3y_3z_3)$ frame.

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

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:

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

Relation (5) can be written as:

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

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

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

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

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

$$\overrightarrow{OM'} = x_1'\vec{e}_{x_1} + y_1'\vec{e}_{y_1} + z_1'\vec{e}_{z_1} = x_3'\vec{e}_{x_3} + y_3'\vec{e}_{y_3} + z_3'\vec{e}_{z_3}. \tag{9}$$

Finally, we obtain that:

$$\begin{aligned}\begin{pmatrix} x_1' \\ y_1' \\ z_1' \end{pmatrix} &= M_1(\theta, \varphi) \begin{pmatrix} x_3' \\ y_3' \\ z_3' \end{pmatrix} \\ &= M_1(\theta, \varphi) M_2(\omega) \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \end{aligned}$$

$$\begin{pmatrix} x_1' \\ y_1' \\ z_1' \end{pmatrix} = M_1(\theta, \varphi) M_2(\omega) M_1(\theta, \varphi)^T \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} \tag{10}$$

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

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

2.1.5. Molien function theory The Haar measure for the SO(3) Lie group is given for function f by the integral:

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

with 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 $\omega \in [0,\pi]$ defines an equivalence class, all the rotations with the same angle but different rotation axes belong to the same class. The character $\chi^{(L)}$ is equal to:

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

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

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

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

$$D\left(\varphi,\theta,\omega\right) = \begin{pmatrix} M\left(\varphi,\theta,\omega\right) & 0 & \cdots & 0 \\ 0 & M\left(\varphi,\theta,\omega\right) & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & M\left(\varphi,\theta,\omega\right) \end{pmatrix} \tag{13}$$

One easily finds that

$$\det\left(I-\lambda D\left(\varphi,\theta,\omega\right)\right) = \left[(1-\lambda)(1-2\lambda\cos\omega+\lambda^2)\right]^N. \tag{14}$$

Collins and Parsons [3] computed 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 (theirs and ours) 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.

2.1.6. Generating functions for the (L) *covariants* For any L, denoting by Γ_N the initial representation of SO(3) on N spatial vectors, we have,

$$\begin{aligned} & g\left((L)\leftarrow\Gamma_N;\lambda\right) \\ &= \frac{1}{2\pi^2}\int_0^{\pi}\int_0^{2\pi}\int_0^{\pi} \frac{\frac{\sin\left(L+\frac{1}{2}\right)\omega}{\sin\frac{\omega}{2}}}{\left[(1-\lambda)(1-2\lambda\cos\omega+\lambda^2)\right]^N}\sin\theta d\theta d\varphi \sin^2\frac{\omega}{2}d\omega \\ &= \frac{2}{\pi}\frac{1}{(1-\lambda)^N}\int_0^{\pi}\frac{\left[\sin\left(L+\frac{1}{2}\right)\omega\right]\sin\frac{\omega}{2}}{(1-2\lambda\cos\omega+\lambda^2)^N}d\omega \end{aligned} \tag{15}$$

the Molien function integral can be simplified by noting that,

$$\left[\sin\left(L+\frac{1}{2}\right)\omega\right]\sin\frac{\omega}{2}=\frac{\cos\left(L\omega\right)-\cos\left[\left(L+1\right)\omega\right]}{2}, \tag{16}$$

so that,

$$\begin{aligned}
&g\left((L)\leftarrow\Gamma_N;\lambda\right)\\
&=\frac{1}{(1-\lambda)^N}\left\{\frac{1}{\pi}\int_0^\pi\frac{\cos\left(L\omega\right)\,d\omega}{(1-2\lambda\cos\omega+\lambda^2)^N}-\frac{1}{\pi}\int_0^\pi\frac{\cos\left[\left(L+1\right)\omega\right]\,d\omega}{(1-2\lambda\cos\omega+\lambda^2)^N}\right\}\\
&=\frac{1}{(1-\lambda)^N}\left(\tilde{g}^{\mathrm{SO}(2)}\left(\widetilde{(L)}\leftarrow\tilde{\Gamma}_N;\lambda\right)-\tilde{g}^{\mathrm{SO}(2)}\left(\widetilde{(L+1)}\leftarrow\tilde{\Gamma}_N;\lambda\right)\right),
\end{aligned} \tag{17}$$

where the tilde quantitites refer to the SO(2) group: $\widetilde{(m)}$, $m\in\mathbb{Z}$ is an irreducible representation of SO(2) and $\tilde{\Gamma}_N$ is the representation generated by N two dimensional vectors. General expressions for $\tilde{g}^{\mathrm{SO}(2)}\left(\widetilde{(L)}\leftarrow\tilde{\Gamma}_N;\lambda\right)$ can be found in [1] or derived from the following formula [4],

$$\begin{aligned}
&\int_0^\pi\frac{\cos nx\,dx}{\left(1-2a\cos x+a^2\right)^m}\\
&=\frac{a^{2m+n-2}\pi}{\left(1-a^2\right)^{2m-1}}\sum_{k=0}^{m-1}\left(\begin{array}{c}m+n-1\\k\end{array}\right)\left(\begin{array}{c}2m-k-2\\m-1\end{array}\right)\left(\frac{1-a^2}{a^2}\right)^k,\quad a^2<1.
\end{aligned} \tag{18}$$

2.2. One spatial vector

Combining the general Molien function formula (17) with Eq.(18) for the case $N=1$, we obtain,

$$g_1\left((L)\leftarrow\Gamma_1;\lambda\right)=\frac{\lambda^L}{1-\lambda^2}. \tag{19}$$

Remark: The sum over L of $g_1\left((L)\leftarrow\Gamma_1;\lambda\right)$ weighted with their order of degeneracy, is equal to $\frac{1}{(1-\lambda)^3}$:

$$\sum_{L=0}^{\infty}\left(2L+1\right)g_1\left((L)\leftarrow\Gamma_1;\lambda\right)=\frac{1}{(1-\lambda)^3}. \tag{20}$$

This relationship can be generalized for every value of N,

$$\sum_{L=0}^{\infty}\left(2L+1\right)g\left((L)\leftarrow\Gamma_N;\lambda\right)=\frac{1}{(1-\lambda)^{3N}}. \tag{21}$$

It simply means that by summing over all symmetry-adapted generating functions with their order of degeneracy one recovers the generating function for the total number of linearly independent polynomials in $3N$ variables of a given degree.

2.3. Two spatial vectors

The six coordinates $\{x_1, y_1, z_1, x_2, y_2, z_2\}$ of two spatial vectors span a six–dimensional representation: $\{x_1, y_1, z_1, x_2, y_2, z_2\}$ that is a direct sum:
$\Gamma_2 = \Gamma_1 \oplus \Gamma_1$. Rather than making use of Eqs. (17) and (18), the generating functions for two vectors can be deduced by coupling the generating functions for one vector obtained in (19), see Appendix A. Distinguishing the two Γ_1 Molien functions by their variables, one obtains:

$$g_1\left((L) \leftarrow \Gamma_2; \lambda_1, \lambda_2\right) = \frac{\sum_{i=0}^{L} \lambda_1^i \lambda_2^{L-i} + \lambda_1\lambda_2 \sum_{i=0}^{L-1} \lambda_1^i \lambda_2^{L-i-1}}{(1-\lambda_1^2)\,(1-\lambda_2^2)\,(1-\lambda_1\lambda_2)}, \tag{22}$$

(with the convention that the second term in the numerator is zero for $L = 0$), or indistinguishing the Γ_1 representation origins by setting $\lambda_1 = \lambda_2 = \lambda$,

$$g_1\left((L) \leftarrow \Gamma_2; \lambda\right) = \frac{(L+1)\lambda^L + L\lambda^{L+1}}{(1-\lambda^2)^3}. \tag{23}$$

2.4. Three spatial vectors

The initial representation $\Gamma_3 = \Gamma_1 \oplus \Gamma_1 \oplus \Gamma_1$ contains nine variables and is reducible. Again, the generating functions for three vectors can be obtained by coupling the generating function for one vector and the generating function for two vectors, according to Appendix A. One obtains the following expression:

$$g_1\left((L) \leftarrow \Gamma_3; \lambda\right) = \frac{\mathcal{N}_1\left((L) \leftarrow \Gamma_3; \lambda\right)}{(1-\lambda^2)^6}, \tag{24}$$

$$\begin{aligned} \mathcal{N}_1\left((L) \leftarrow \Gamma_3; \lambda\right) = {}& \frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} \\ & - (L+1)(L-1)\lambda^{L+3} - \frac{L(L-1)}{2}\lambda^{L+4}. \end{aligned} \tag{25}$$

The coefficients in the numerator (24) 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 (26).

$$\begin{aligned} g_2\left((L) \leftarrow \Gamma_3; \lambda\right) = {}& \frac{(2L+1)\lambda^L + (2L+1)\lambda^{L+1}}{(1-\lambda^2)^6} \\ & + \frac{\frac{L(L-1)}{2}\lambda^L + (L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}}{(1-\lambda^2)^5}, \end{aligned} \tag{26}$$

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 a generalized integrity basis are given in Table 1 up to $L = 6$.

Table 1. Expressions of the symbolically interpretable g_i Molien functions for three spatial vectors and (L) final irreducible representations, $0 \le L \le 6$.

i	Γ_{final}	$g_i\left(\Gamma_{\text{final}} \leftarrow \Gamma_3; \lambda\right)$
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	$\vdots$	$\vdots$

We have proceeded in a similar fashion to obtain the generating function for four and five spatial vectors given in Appendix B.1 and Appendix B.2 respectively. Any number of spatial vectors can be achieved by recursion, in principle.

2.5. Extension to O(3)

The block matrix representation of the inversion operation for the Γ_N initial representation is $-I_{3N}$, where I_{3N} is the $3N \times 3N$ identity matrix. So, denoting by $(L)^\epsilon, \epsilon = \pm$, the irreducible representations of O(3), the corresponding Molien functions are easily obtained:

$$g^{\mathrm{O}(3)}\left((L)^\epsilon \leftarrow \Gamma_N; \lambda\right) = \frac{1}{2}\left[g\left((L) \leftarrow \Gamma_N; \lambda\right) + \epsilon g\left((L) \leftarrow \Gamma_N; -\lambda\right)\right].$$

3. Two conjectures around the Molien function

3.1. First conjecture

Based on the results of the previous section, we conjecture that for any number of three dimensional vectors and any final representation of SO(3), there exists a positive integer $l_{\max}(N, L)$ with $1 \leq l_{\max}(N, L) \leq 3N - 2$, such that the Molien function g can be cast in the form of a sum of rational fractions:

$$g\left((L) \leftarrow \Gamma_N; \lambda\right) = \sum_{l=1}^{l_{\max}(N,L)} \frac{\mathcal{N}^l_{N,L}(\lambda)}{\left(1-\lambda^2\right)^{3N-2-l}}, \tag{27}$$

with the $l_{\max}(N, L)$ numerator polynomials $\mathcal{N}^l_{N,L}(\lambda) = \sum\limits_{n=0}^{n_{\max}(N,L,l)} c^{l,n}_{N,L} \lambda^{L+n}$ having only non–negative coefficients $c^{l,n}_{N,L}$. The exponents on λ in the numerator polynomials start at L, since (L)–covariants built from vectors are at least of total degree L.

The ring of invariant polynomials ($L = 0$) under the reductive SO(3) group is a free module over a subring of invariant polynomials [5, 6]. It admits an homogeneous system of parameters or Hironaka decomposition and the Molien function for invariant polynomials can be cast in the form (27) with a single rational fraction. Its symbolic interpretation suggests $3N - 3$ primary or denominator invariant polynomials of degree 2 and $c^{1,n}_{N,0}$ secondary or numerator invariant polynomials of degree $L + n$ with $0 \leq n \leq n_{\max}(N, 0, 1)$.

If the module of (L)–covariants ($L > 0$) is free, the situation is similar to the ring of invariant polynomials: the form (27) is a single rational fraction and the usual Molien function interpretation in terms of integrity basis holds. If the module of (L)–covariants is not free, and this can happen [7], then $l_{\max} > 1$. The form (27) admits a symbolic interpretation in terms of a generalized integrity basis already proposed in our previous work on SO(2) [1]. The non free module is a sum of $l_{\max}(N, L)$ submodules. Each of these submodules is a free module that corresponds to the l^{th} rational fraction symbolic interpretation in terms of integrity basis ($1 \leq l \leq l_{\max}(N, L)$): it is a module on a ring of invariants generated by $3N - 2 - l$ primary invariants and the minimal number of covariant generators of degree $L+n$ is given by $c^{l,n}_{N,L}$. So, this conjecture is in fact closely related to that of Stanley: conjecture 5.1 of Ref. [8].

In practice, the numerators in the sum of expression (27) can be determined algorithmically for a given pair (N, L) by starting with the $g_1\left((L) \leftarrow \Gamma_N; \lambda\right)$ expression, which is always a single rational fraction. If for the value of L considered, the numerator $\mathcal{N}_1$ has only non–negative coefficients, then the form is the desired one and the algorithm stops. Otherwise we perform a polynomial long division of the numerator by $1 - \lambda^2$. The division process is stopped not when the degree of the remainder r_1 is less than 2 as one would do in the usual Euclidean polynomial division, but when the coefficients of the remainder r_1 become non–negative for the L-value considered, which will happen according to the conjecture. Then the numerator is rewritten as:

$$\mathcal{N}_1 = r_1 + \left(1-\lambda^2\right) q_1.$$

The remainder r_1 serves as the numerator of the first rational fraction in (27). If the quotient q_1 has only non–negative coefficients for the value of L considered, the algorithm stops and the final form of the Molien function is then:

$$g\left((L) \leftarrow \Gamma_N;\lambda\right) = \frac{r_1}{\left(1-\lambda^2\right)^{3N-3}} + \frac{q_1}{\left(1-\lambda^2\right)^{3N-4}}.$$

Otherwise, the process is iterated, *i.e.* the quotient q_1 is divided in the same way by $1-\lambda^2$ and the new remainder will constitute the numerator of the second rational fraction. The procedure is repeated until the quotient has also only non–negative coefficients, which will happen according to the conjecture.

For example, for $N=3$, the single rational fraction (24) with its numerator (25) is suitable for $L<2$. For $L\geq 2$, we obtain successively by the division process of the numerator (25):

$$\begin{aligned}
&\frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} - (L+1)(L-1)\lambda^{L+3} - \frac{L(L-1)}{2}\lambda^{L+4} \\
&= (1-\lambda^2)\left(\frac{L(L-1)}{2}\lambda^{L+2}\right) + \frac{(L+2)(L+1)}{2}\lambda^L + (L+2)L\lambda^{L+1} - \frac{L(L-1)}{2}\lambda^{L+2} - (L+1)(L-1)\lambda^{L+3} \\
&= (1-\lambda^2)\left((L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}\right) + \frac{(L+2)(L+1)}{2}\lambda^L + (2L+1)\lambda^{L+1} - \frac{L(L-1)}{2}\lambda^{L+2} \\
&= (1-\lambda^2)\left(\frac{L(L-1)}{2}\lambda^L + (L+1)(L-1)\lambda^{L+1} + \frac{L(L-1)}{2}\lambda^{L+2}\right) + (2L+1)\lambda^L + (2L+1)\lambda^{L+1}
\end{aligned} \tag{28}$$

The remainder $(2L+1)\lambda^L + (2L+1)\lambda^{L+1}$ has only non negative coefficients and is the numerator of the first rational 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 $L\geq 2$. It will constitute the numerator of the second fraction and we find again the expression (26) with two rational fractions for the Molien function.

For $N=4$, the numerator expression $\mathcal{N}_1\left((L)\leftarrow\Gamma_4;\lambda\right)$ is suitable for $L<3$. For $L\geq 3$, we obtain successively by the division process of the initial numerator:

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

$$+\frac{(L+3)(L+2)L}{2}\lambda^{L+1}+\frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2}-\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3}-\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+4}$$
$$=(1-\lambda^2)\left(\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}\right)$$
$$+\frac{(L+3)(L+2)(L+1)}{6}\lambda^{L}+\frac{(L+3)(L+2)L}{2}\lambda^{L+1}-\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2}-\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3}$$
$$=(1-\lambda^2)\left(\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}\right)$$
$$+\frac{(L+3)(L+2)(L+1)}{6}\lambda^{L}+\frac{(L+3)(L+2)L}{2}\lambda^{L+1}-\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2}-\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+3}$$
$$=(1-\lambda^2)\left(\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}\right.$$
$$\left.-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}\right)+\frac{(L+3)(L+2)(L+1)}{6}\lambda^{L}+4(2L+1)\lambda^{L+1}-\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L+2} \tag{29}$$
$$=(1-\lambda^2)\left(\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L}+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}\right.$$
$$\left.-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}\right)+4(2L+1)\lambda^{L}+4(2L+1)\lambda^{L+1} \tag{30}$$

For $L=3$ and $L=4$, the algorithm stops at Eq. (29), where all coefficients of the remainder are positive, whereas for larger values of L the coefficient $-\frac{(L^3+6L^2-37L-18)}{6}$ of λ^{L+2} is negative in the remainder of Eq. (29) and one must stop only at Eq. (30). Let us consider first the cases $L=3$ and $L=4$. The quotient has negative coefficients and must be divided again by $(1-\lambda^2)$,

$$\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}$$
$$=(1-\lambda^2)\left(\frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right)+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{2}\lambda^{L+3}$$
$$-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}$$
$$=(1-\lambda^2)\left(\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2}+\frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right)+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}-\frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2}$$
$$-\frac{L(L-1)(L-2)}{2}\lambda^{L+3}$$
$$=(1-\lambda^2)\left(\frac{L(L-1)(L-2)}{2}\lambda^{L+1}+\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2}+\frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right)+2(L-2)(2L+1)\lambda^{L+1}$$
$$-\frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2} \tag{31}$$

This time both remainder and quotient have non negative coefficients, so we stop here and retrieve the numerators of the second and third fractions of g_2 in Eq. (B.3). For $L>4$, we have to divide the quotient of Eq. (30) by $(1-\lambda^2)$,

$$\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L}+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}-\frac{L(L-1)(L-2)}{3}\lambda^{L+3}$$
$$-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}-\frac{L(L-1)(L-2)}{6}\lambda^{L+5}$$
$$=(1-\lambda^2)\left(\frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right)+\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L}+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}+\frac{(L-2)(L^2+8L+3)}{3}\lambda^{L+2}$$
$$-\frac{L(L-1)(L-2)}{2}\lambda^{L+3}-\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+4}$$
$$=(1-\lambda^2)\left(\frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2}+\frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right)+\frac{(L^3+6L^2-37L-18)}{6}\lambda^{L}+\frac{(L-2)(L^2+7L+4)}{2}\lambda^{L+1}$$

$$
\begin{aligned}
&\qquad - \frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2} - \frac{L(L-1)(L-2)}{2}\lambda^{L+3} \\
&= (1-\lambda^2)\left(\frac{L(L-1)(L-2)}{2}\lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right) + \frac{(L^3+6L^2-37L-18)}{6}\lambda^{L} \\
&\qquad + 2(L-2)(2L+1)\lambda^{L+1} - \frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2} \qquad (32) \\
&= (1-\lambda^2)\left(\frac{(L-2)(L^2-16L-9)}{6}\lambda^{L} + \frac{L(L-1)(L-2)}{2}\lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}\right) \\
&\qquad + 2(L-3)(2L+1)\lambda^{L} + 2(L-2)(2L+1)\lambda^{L+1} \qquad (33)
\end{aligned}
$$

For $5 \leq L \leq 16$ one stops at Eq. (32), where all coefficients of the remainder are positive, whereas for larger values of L the coefficient of λ^{L+2} is negative in the remainder of Eq. (32) and one must continue up to Eq. (33). In both cases, the quotient has only non-negative coefficients, so the remainders and quotients of Eqs. (32) and (33) gives the numerators of the second and third fractions of g_3 and g_4 in Eqs. (B.4) and (B.5). We leave it to the reader to treat the case $N = 5$.

3.2. Conjecture 2

For the electric dipole moment hypersurface, the relevant covariant module corresponds to the (1) irreducible representation and will always be a free module. This conjecture is based on the observation that for a given N, $g_1\left((L) \leftarrow \Gamma_N; \lambda\right)$ has the right form of Eq. (27) for all L if $N = 1$ or $N = 2$ and for all $L < N$ if $5 \geq N > 2$.

4. Construction of the generating families for N vectors

The main goal of this section, is to propose a general method to obtain a suitable generating family of SO(3) covariants in the case of non-free module. This method takes advantage of the interpretable form of the Molien function seen in the previous section. The simplest case of a non-free module occurs for $N = 3$ vectors and $L = 2$. We will first provide explicit, natural basis sets for the free cases corresponding to $N \in \{1, 2\} L \in \{0, 1, 2\}$ and $N = 3, L \in \{0, 1\}$. Then, we will show how to deal with the simplest non-free case: $N = 3, L = 2$. Finally, we will explain how to generalize the latter construction.

4.1. One spatial vector

The initial representation Γ_1 contains the three variables x_1, y_1, z_1, and Eq. 19 shows that there is one basic invariant of order 2, and one set of $(2L+1)$-degenerate auxiliary covariants of order L spanning the (L)-covariant free module.

The basic invariant is of course the scalar product $Q_{11} = x_1^2 + y_1^2 + z_1^2$, while the auxiliary covariants are spherical harmonics. For example, for $L = 1$ one can take the set $\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$, for $L = 2$, $\begin{pmatrix} 2z_1^2 - x_1^2 - y_1^2 \\ x_1 z_1 \\ y_1 z_1 \\ x_1 y_1 \\ x_1^2 - y_1^2 \end{pmatrix}$, and so on.

4.2. Two spatial vectors

The ring of invariant is well-known [9] and generated by the 3 scalar products: $Q_{11} = x_1^2 + y_1^2 + z_1^2$, $Q_{22} = x_2^2 + y_2^2 + z_2^2$, $Q_{12} = x_1 x_2 + y_1 y_2 + z_1 z_2$.

For $L = 1$,

$$g_1\left((1) \leftarrow \Gamma_2; \lambda_1, \lambda_2\right) = \frac{\lambda_1 + \lambda_2 + \lambda_1\lambda_2}{(1-\lambda_1^2)\,(1-\lambda_2^2)\,(1-\lambda_1\lambda_2)}. \tag{34}$$

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 $\begin{pmatrix} y_1 z_2 - z_1 y_2 \\ z_1 x_2 - x_1 z_2 \\ x_1 y_2 - y_1 x_2 \end{pmatrix}$.

$$g_1^{\mathrm{O}(3)}\left((1^-) \leftarrow \Gamma_2^{\mathrm{O}(3)}; \lambda\right) = \frac{2\lambda}{(1-\lambda^2)^3}. \tag{35}$$

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

$$DMS[x_1, y_1, z_1, x_2, y_2, z_2] = P_{z_1}[Q_{11}, Q_{22}, Q_{12}] z_1 + P_{z_2}[Q_{11}, Q_{22}, Q_{12}] z_2, \tag{36}$$

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

For $L = 2$,

$$g_1\left((2) \leftarrow \Gamma_2; \lambda_1, \lambda_2\right) = \frac{\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2 + \lambda_1^2\lambda_2 + \lambda_1\lambda_2^2}{(1-\lambda_1^2)\,(1-\lambda_2^2)\,(1-\lambda_1\lambda_2)}. \tag{37}$$

The three second order (2)-covariant basis vectors can be guessed as $\begin{pmatrix} 2z_1^2 - x_1^2 - y_1^2 \\ x_1 z_1 \\ y_1 z_1 \\ x_1 y_1 \\ x_1^2 - y_1^2 \end{pmatrix}$,

$\begin{pmatrix} 2z_2^2-x_2^2-y_2^2 \\ x_2z_2 \\ y_2z_2 \\ x_2y_2 \\ x_2^2-y_2^2 \end{pmatrix}$ and $\begin{pmatrix} 2z_1z_2-x_1x_2-y_1y_2 \\ x_1z_2+z_1x_2 \\ y_1z_2+z_1y_2 \\ x_1y_2+y_1x_2 \\ x_1x_2-y_1y_2 \end{pmatrix}$, by analogy with spherical harmonics and the two third order ones can be constructed by subtituting one set of coordinates in the last expression by the $(L=1)$-cross-product covariant,

$$\begin{pmatrix} 2z_1(x_1y_2-y_1x_2)-x_1(y_1z_2-z_1y_2)-y_1(z_1x_2-x_1z_2) \\ x_1(x_1y_2-y_1x_2)+z_1(y_1z_2-z_1y_2) \\ y_1(x_1y_2-y_1x_2)+z_1(z_1x_2-x_1z_2) \\ x_1(z_1x_2-x_1z_2)+y_1(y_1z_2-z_1y_2) \\ x_1(y_1z_2-z_1y_2)-y_1(z_1x_2-x_1z_2) \end{pmatrix},$$

$$\begin{pmatrix} 2(x_1y_2-y_1x_2)z_2-(y_1z_2-z_1y_2)x_2-(z_1x_2-x_1z_2)y_2 \\ (y_1z_2-z_1y_2)z_2+(x_1y_2-y_1x_2)x_2 \\ (z_1x_2-x_1z_2)z_2+(x_1y_2-y_1x_2)y_2 \\ (y_1z_2-z_1y_2)y_2+(z_1x_2-x_1z_2)x_2 \\ (y_1z_2-z_1y_2)x_2-(z_1x_2-x_1z_2)y_2 \end{pmatrix}.$$

4.3. Three spatial vectors

The ring of invariant is well-known [9] and generated by the 6 scalar products: $Q_{ij} := x_ix_j+y_iy_j+z_iz_j$ for $1 \le i \le j \le 3$.
For $L=0$,

$$g_1\left((0) \leftarrow \Gamma_3; \lambda_1, \lambda_2, \lambda_3\right) = \frac{1+\lambda_1\lambda_2\lambda_3}{\left(1-\lambda_1^2\right)\left(1-\lambda_2^2\right)\left(1-\lambda_1\lambda_2\right)\left(1-\lambda_1\lambda_3\right)\left(1-\lambda_2\lambda_3\right)}, \tag{38}$$

the secondary invariants are the scalar 1 and the determinant $\begin{vmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{vmatrix}$

For $L=1$,

$$g_1\left((1) \leftarrow \Gamma_3; \lambda_1, \lambda_2, \lambda_3\right) = \frac{\lambda_1+\lambda_2+\lambda_3+\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3}{\left(1-\lambda_1^2\right)\left(1-\lambda_2^2\right)\left(1-\lambda_1\lambda_2\right)\left(1-\lambda_1\lambda_3\right)\left(1-\lambda_2\lambda_3\right)}. \tag{39}$$

The three first order (1)-covariant basis vectors can be taken as $\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$, $\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$ and $\begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix}$, and the three second order one as their cross-product $\begin{pmatrix} y_1z_2-z_1y_2 \\ z_1x_2-x_1z_2 \\ x_1y_2-y_1x_2 \end{pmatrix}$, $\begin{pmatrix} y_1z_3-z_1y_3 \\ z_1x_3-x_1z_3 \\ x_1y_3-y_1x_3 \end{pmatrix}$, $\begin{pmatrix} y_2z_3-z_2y_3 \\ z_2x_3-x_2z_3 \\ x_2y_3-y_2x_3 \end{pmatrix}$.

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

$$\begin{aligned} DMS[x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3] = P_{z_1}[(Q_{ij})_{1\le i\le j\le 3}] \times z_1 + P_{z_2}[(Q_{ij})_{1\le i\le j\le 3}] \times z_2 \\ + P_{z_3}[(Q_{ij})_{1\le i\le j\le 3}] \times z_3 + P_{x_1y_2-y_1x_2}[(Q_{ij})_{1\le i\le j\le 3}] \times (x_1y_2 - y_1x_2) + \\ P_{x_1y_3-y_1x_3}[(Q_{ij})_{1\le i\le j\le 3}] \times (x_1y_3 - y_1x_3) + P_{x_2y_3-y_2x_3}[(Q_{ij})_{1\le i\le j\le 3}] \times (x_2y_3 - y_2x_3), \end{aligned} \tag{40}$$

where the P_i's are polynomials in the primary invariants. The other components are related by symmetry.

For $L = 2$, when the representations are distinguished, the symbolic interpretation of the numerator of the Molien function,

$$\begin{aligned} \mathcal{N}_1\left((2) \leftarrow \Gamma_3; \lambda_1, \lambda_2, \lambda_3\right) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 + \\ \lambda_1^2\lambda_2 + \lambda_1^2\lambda_3 + \lambda_1\lambda_2^2 + \lambda_1\lambda_3^2 + \lambda_2^2\lambda_3 + \lambda_2\lambda_3^2 + 2\lambda_1\lambda_2\lambda_3 \\ - \lambda_1^2\lambda_2^2\lambda_3 - \lambda_1^2\lambda_2\lambda_3^2 - \lambda_1\lambda_2^2\lambda_3^2 - \lambda_1^2\lambda_2^2\lambda_3^2 \end{aligned} \tag{41}$$

suggests that there are 6 linearly independent, auxiliary covariants of order 2 and 8 of order 3 related by 3 syzygies of order 5 and 1 of order 6. Then, the symbolic interpretation of

$$g_2\left((2) \leftarrow \Gamma_3; \lambda\right) = \frac{5\lambda^2 + 5\lambda^3}{(1-\lambda^2)^6} + \frac{\lambda^2 + 3\lambda^3 + \lambda^4}{(1-\lambda^2)^5}. \tag{42}$$

specifies that only 5 auxiliary covariants of order 2 and 5 of order 3 should be used to generate a free module over the whole ring (associative algebra) of primary invariants $\mathcal{A}$, denoted $\mathcal{M}_1^{\mathcal{A}}$. However, to generate the $N = 3, L = 2$ covariant module, this free module should be completed by a second one, $\mathcal{M}_2^{\tilde{\mathcal{A}}}$, spanned by one auxiliary covariant of order 2, three of order 3 and one of order 4, over a subring (subalgebra) $\tilde{\mathcal{A}}$ spanned by only five primary invariants.

Let us exploit these pieces of information. For $1 \le i \le j \le 3$, we define

$$D_{ij} := 2z_i * z_j - x_ix_j - y_iy_j. \tag{43}$$

From the well-known expressions of spherical harmonics, we deduce that the D_{ij}'s are the $(m_L = 0)$-components of the 6 auxiliary covariants of order 2, we are looking for. Let us further construct a similar expression by substituting an order 1 by an order 2 $(L = 1)$-covariant,

$$\forall i,j,k \in \{1,2,3\} \quad T_{ijk} := 2z_i\left(x_jy_k - x_ky_j\right) - x_i\left(y_jz_k - y_kz_j\right) - y_i\left(x_kz_j - x_jz_k\right). \tag{44}$$

The T_{ijk}'s are the $(m_L = 0)$-components of order 3 covariants. However, only 8 can be linearly independent, since $\forall i,j,k \in \{1,2,3\}$ $T_{ijk} + T_{ikj} = 0$ and $T_{ijk} + T_{jki} + T_{kij} = 0$.

For a given i, we retain only those T_{ijk} with $j < k$, and for i, j, k all distinct, we decide to discard

$$T_{213} = T_{123} + T_{312}. \tag{45}$$

The three syzygies of order 5 are found to be, by solving linear systems of equations:

$$Q_{23} * T_{112} - Q_{22} * T_{113} - Q_{13} * T_{212} - Q_{11} * T_{223} + Q_{12} * (2 * T_{123} + T_{312}) = 0 \tag{46}$$

$$Q_{13} * T_{223} + Q_{33} * T_{212} - Q_{12} * T_{323} + Q_{22} * T_{313} - Q_{23} * (2 * T_{312} + T_{123}) = 0 \tag{47}$$

$$Q_{11} * T_{323} + Q_{23} * T_{113} - Q_{12} * T_{313} - Q_{33} * T_{112} + Q_{13} * (2 * T_{312} - T_{213}) = 0 \tag{48}$$

the last one can be rewritten by using Eq.(45) as

$$Q_{11} * T_{323} + Q_{23} * T_{113} - Q_{12} * T_{313} - Q_{33} * T_{112} + Q_{13} * (T_{312} - T_{123}) = 0. \tag{49}$$

Similarly, the syzygie of order 6 is found to be:

$$\begin{aligned}&(Q_{23}^2 - Q_{22} * Q_{33}) * D_{11} + (Q_{13}^2 - Q_{11} * Q_{33}) * D_{22} + (Q_{12}^2 - Q_{11} * Q_{22}) * D_{33} + \\ &2 * ((Q_{12} * Q_{33} - Q_{13} * Q_{23}) * D_{12} + (Q_{13} * Q_{22} - Q_{12} * Q_{23}) * D_{13} + (Q_{11} * Q_{23} - Q_{12} * Q_{13}) * D_{23}) = 0\end{aligned} \tag{50}$$

There is some arbitrariness in the choice of the primary invariant to be removed from the invariant ring $\mathcal{A}$ to define $\mathcal{M}_2^{\tilde{\mathcal{A}}}$. Let us choose Q_{23}, so that $\tilde{\mathcal{A}}$ is the subring of $\mathcal{A}$ spanned by $\{Q_{11}, Q_{22}, Q_{33}, Q_{12}, Q_{13}\}$. Then, the natural order 2 auxiliary covariant to be eliminated from $\mathcal{M}_1^{\mathcal{A}}$ is D_{11}, since including it in $\mathcal{M}_2^{\tilde{\mathcal{A}}}$, together with the order 4 covariant, $Q_{23} \times D_{11}$ is sufficient to obtain all the $(Q_{23}^n \times D_{11})$'s with $n > 1$. This results from Eq.(50), which permits to reexpress $Q_{23}^2 \times D_{11}$ in terms of other elements of the $\mathcal{M}_2^{\tilde{\mathcal{A}}}$ module. It remains to select the three order 3 auxiliary covariants to exclude from $\mathcal{M}_1^{\mathcal{A}}$ and include in $\mathcal{M}_2^{\tilde{\mathcal{A}}}$. The natural choice is T_{112}, $(2 * T_{123} + T_{123})$ and T_{113}, since $Q_{23} * T_{112}$, $Q_{23} * (2 * T_{123} + T_{123})$ and $Q_{23} * T_{113}$, are easily re-expressed with terms either in $\mathcal{M}_1^{\mathcal{A}}$ or in $\mathcal{M}_2^{\tilde{\mathcal{A}}}$, by means of the syzygies Eqs.(46), (47) and (49) respectively. The 5 order 2 auxilliary covariants and the 5 order 3 auxilliary covariants spanning $\mathcal{M}_1^{\mathcal{A}}$ can be chosen to be $D_{12}, D_{13}, D_{22}, D_{23}, D_{33}, T_{123}, T_{212}, T_{223}, T_{313}, T_{323}$.

4.4. Generalization to higher N and L values

The path followed in the previous section for $N = 3$ and $L = 2$ can be generalized to higher values of N and L. The decomposition of non-free modules into a sum of free modules on subrings of the ring of primary invariants will have more terms: Table B1 suggests 3-term decompositions for $N = 4$ and $L \geq 3$, while Table B2 suggests 4-term decompositions for $N = 5$ and $L \geq 4$. One is tempted to conjecture that $(N-1)$-term decompositions will occur for N-vectors and $L \geq N - 1$, for all $N \geq 2$. The decompositions are not unique, since, as we have seen, there is some arbitrariness in the choice of the generators of the primary invariant subrings and of the covariant generators of the modules on these subrings (although some choices are more natural than others). So, it is difficult to give a general and explicit construction. We only sketch the main line.

The construction follows the steps of the algorithm of section 3.1. The number of covariant generators of each degree for each free module in the decomposition: $\mathcal{M}_1^{\tilde{\mathcal{A}}^0}$, $\mathcal{M}_2^{\tilde{\mathcal{A}}^1}$, $\mathcal{M}_3^{\tilde{\mathcal{A}}^2}$, …, (where $\tilde{\mathcal{A}}^0 = \mathcal{A}$, $\tilde{\mathcal{A}}^1 = \tilde{\mathcal{A}}$ in our previous notation) are given by the successive rests of the divisions by $(1-\lambda^2)$ and the last quotient with only positive coefficients. To find successive sets of syzygies, it suffices to solve linear systems in the primary invariant ring and its successively selected subrings. The numbers of independent syzygies to obtain and their degrees, are given by the negative coefficients in the expressions of the numerator $\mathcal{N}_1$ and its successive quotients by $(1-\lambda^2)$ appearing while following the algorithm of section 3.1. For example, for $N = 4, L = 3$, Eq.(B.2) tells us that there will be 19 syzygies of degree 6 and 16 of degree 7 to be used in order to select $\tilde{\mathcal{A}}^1$ and the 20 generators of degree 3, 28 generators of degree 4 and 48 generators of degree 5 of $\mathcal{M}_1^{\tilde{\mathcal{A}}^0}$ according to the rest in Eq.(29). This first set of syzygies is to be obtained by solving a linear system in $\mathcal{A}$. Then, the quotient of Eq.(29) tells us that a second set of 2 syzygies of degree 6, 4 of degree 7 and 1 of degree 8 is to be obtained by solving linear systems in the subring $\tilde{\mathcal{A}}^1$, previously selected. Finally, the rest in Eq.(31), tells us that there are 14 covariant generators of degree 4 and 8 of degree 5 to be chosen for $\mathcal{M}_2^{\tilde{\mathcal{A}}^1}$, and the quotient in Eq.(31) that, once $\tilde{\mathcal{A}}^2$ has been selected, there will be 3 covariant generators of degree 4, 4 of degree 5 and 1 of degree 6 to be found for $\mathcal{M}_3^{\tilde{\mathcal{A}}^2}$.

Since the $\mathcal{S}_N$ permutation group action on vector indices preserves partial degrees, one can take advantages of the Molien functions with distinguished representation arguments, to obtain information about the partial degrees of the variables in these syzygies. This reduces significantly the size of the linear systems to be solved. For example, in the $N = 3$ and $L = 2$ case, the syzygie of order 6 is found to be of partial degrees $n_1 = n_2 = n_3 = 2$ from the last term in Eq.(41). Though, we have not systematically reported such detailed expressions for $N > 2$, because the closed formulas we have obtained are not polynomial. For example, for $N = 3$, we have obtained the following fraction

$$\begin{aligned}\mathcal{N}_1\left((L) \leftarrow \Gamma_3; \lambda_1, \lambda_2, \lambda_3\right) = {} & \frac{1}{(\lambda_1-\lambda_2)(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)}\left[\lambda_2\lambda_3\left(-\lambda_3^{1+L} - \lambda_2\lambda_3^{1+L} + \lambda_2^{1+L}(1+\lambda_3)\right) + \right.\\ & \lambda_1^3\lambda_2\lambda_3\left(-\lambda_3^{1+L} - \lambda_2\lambda_3^{1+L} + \lambda_2^{1+L}(1+\lambda_3)\right) + \lambda_1^{2+L}\left(-\lambda_3(1+\lambda_3) - \lambda_2^3\lambda_3(1+\lambda_3) + \lambda_2\left(1+\lambda_3^3\right) + \right.\\ & \left.\left.\lambda_2^2\left(1+\lambda_3^3\right)\right) + \lambda_1\left(\lambda_3^{2+L} + \lambda_2^3\lambda_3^{2+L} - \lambda_2^{2+L}\left(1+\lambda_3^3\right)\right) + \lambda_1^2\left(\lambda_3^{2+L} + \lambda_2^3\lambda_3^{2+L} - \lambda_2^{2+L}\left(1+\lambda_3^3\right)\right)\right]\end{aligned} \tag{51}$$

which we only managed to simplify into interpretable polynomial expressions such as Eq.(41), when L takes specific values. Such interpretable, detailed expressions can also be exploited to provide the partial degrees of the covariant generators of the modules, after division by the factor in the denominator corresponding to the primary invariant excluded from the next subring in the decomposition.

5. Conclusion

We have derived general expressions of the Molien generating function for N vectors of the three dimensional Euclidian space to compute the number of invariants and covariants of the SO(3) symmetry group. An extension to the O(3) group is easy. In the case where the module of covariant is non free, an algorithm to transform the Molien function into a form amenable to a symbolic interpretation in term of a generalized integrity basis has been proposed. The same algorithm can serve to build step by step such a generalized integrity basis, which consists in a collection of basis of covariants for free covariant modules over subrings of the ring of primary invariants.

The case of the invariant ("$L = 0$ covariants") module, is always free. In quantum physics, an integrity basis can be useful to express SO(3)-totally invariant observables such as the so-called potential energy hypersurface in quantum chemistry [10], when it is not possible or appropriate to separate out rotational from internal coordinates. Note that such an observable is actually O(3)-totally invariant, but for polyatomic molecules of four atoms and more, it is more practical to use coordinates, such as dihedral angles, that are SO(3)- but not O(3)-invariants.

We have conjectured that the $L = 1$ covariants module will always be free, as well. We have provided explicit integrity basis up to $N = 3$. In quantum physics, these integrity basis can be useful to express observables such as dipole moment hypersurface, used in quantum chemistry to calculate dipolar transition intensities. If, in addition to the 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 [10] 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. (36) must satisfy, $P_{z_1}[Q_1, Q_2, Q_3] = P_{z_2}[Q_2, Q_1, Q_3]$, and $P_{x_1y_2-y_1x_2}[Q_1, Q_2, Q_3] = -P_{x_1y_2-y_1x_2}[Q_2, Q_1, Q_3]$.

The $(L = 2)$-case can be useful in theoretical physics and chemistry to expand observables such as quadrupole moments. However, the elimination of some primary invariants breaks the permutational symmetry of the subrings used for the modules $\mathcal{M}_2^{\tilde{A}^1}$, $\mathcal{M}_3^{\tilde{A}^2}$, ..., of the covariant module decomposition. So, unfortunately in such a case, further permutational symmetry adaptation will be unpractical in general.

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References

[1] G. Dhont and B. I. Zhilinskií. 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. König. Preuss. Akad. Wiss.*, 52:1152–1156, 1897.

[3] 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.

[4] I. S. Gradshteyn and I. M. Ryzhik. *Table of Integrals, Series, and Products.* Academic Press, New York, 1980. Equation (3.616.7).

[5] M. Hochster and J. L. Roberts. Rings of invariants of reductive groups acting on regular rings are Cohen–Macaulay. *Adv. Math.*, 13(2):115–175, 1974.

[6] H. Derksen and G. Kemper. *Computational Invariant Theory.* Springer Berlin Heidelberg, Berlin, Heidelberg, 2015.

[7] Michael Van den Bergh. Modules of covariants. In S. D. Chatterji, editor, *Proceedings of the International Congress of Mathematicians*, pages 352–362, Basel, 1995. Birkhäuser Basel.

[8] R. P. Stanley. Linear diophantine equations and local cohomology. *Invent. Math.*, 68(2):175–193, 1982.

[9] H. Weyl. *The Classical Groups. Their Invariants and Representations.* Princeton University Press, Princeton, New Jersey, 1939.

[10] P. Cassam-Chenaï and F. Patras. Symmetry–adapted polynomial basis for global potential energy surfaces-applications to XY_4 molecules. *J. Math. Chem.*, 44(4):938–966, 2008.

[11] L. Michel and B. I. Zhilinskií. Symmetry, invariants, topology. Basic tools. *Phys. Rep.*, 341(1–6):11–84, 2001.

Appendix A. Generating functions obtained by coupling

The Molien function with a direct sum initial representation $g^G\left(\Gamma_{\text{final}} \leftarrow \Gamma_{\text{initial},1} \oplus \Gamma_{\text{initial},2}; \lambda\right)$ can be calculated using Molien functions for the $\Gamma_{\text{initial},1}$ and $\Gamma_{\text{initial},2}$ initial representations, see Eq.(43) of [11]:

$$g^G\left(\Gamma_f \leftarrow \Gamma_{i,1} \oplus \Gamma_{i,2}; \lambda\right) = \sum_{\Gamma_{f,1}} \sum_{\Gamma_{f,2}} n^{\Gamma_f}_{\Gamma_{f,1},\Gamma_{f,2}} g^G\left(\Gamma_{f,1} \leftarrow \Gamma_{i,1}; \lambda\right) g^G\left(\Gamma_{f,2} \leftarrow \Gamma_{i,2}; \lambda\right), \quad \text{(A.1)}$$

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

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

$$\Gamma_N = \Gamma_1 \oplus \Gamma_{N-1},$$

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

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

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

Appendix B. Generating function for four and five vectors

Appendix B.1. Generating function for four vectors

Let us write the four spatial vector generating function in the form,

$$g_1\left((L) \leftarrow \Gamma_4; \lambda\right) = \frac{\mathcal{N}_1\left((L) \leftarrow \Gamma_4; \lambda\right)}{(1-\lambda^2)^9}, \tag{B.1}$$

By coupling the generating function for one vector and the generating function for three vectors, the numerator is found to be:

$$\begin{aligned}
&\mathcal{N}_1\left((L); \Gamma_4; \lambda\right)\\
&= \frac{(L+3)(L+2)(L+1)}{6}\lambda^L + \frac{(L+3)(L+2)L}{2}\lambda^{L+1}\\
&\quad + \frac{(L+3)(L+2)(L+1)}{6}\lambda^{L+2} - \frac{(L+3)(L-2)(5L+4)}{6}\lambda^{L+3}\\
&\quad - \frac{(L+3)(L-2)(5L+1)}{6}\lambda^{L+4} + \frac{L(L-1)(L-2)}{6}\lambda^{L+5}\\
&\quad + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+6} + \frac{L(L-1)(L-2)}{6}\lambda^{L+7}
\end{aligned} \tag{B.2}$$

The generating function (B.1) has positive or null coefficients in its numerators for $L = 0$, 1 or 2. Negative coefficients appear for $L \geq 3$. However, the Molien function can be rewritten as (B.3), which has only positive coefficients for $L = 2$, 3 or 4, as (B.4), which has only positive coefficients for L between 5 and 16, and as (B.5), which has only positive coefficients for $L \geq 17$.

$$\begin{aligned}
&g_2\left((L) \leftarrow \Gamma_4; \lambda\right)\\
&= \frac{\frac{(L+3)(L+2)(L+1)}{6}\lambda^L + 4(2L+1)\lambda^{L+1} + (-\frac{1}{6}L^3 - L^2 + \frac{37}{6}L + 3)\lambda^{L+2}}{(1-\lambda^2)^9}\\
&\quad + \frac{2(L-2)(2L+1)\lambda^{L+1} - \frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2}}{(1-\lambda^2)^8}\\
&\quad + \frac{\frac{L(L-1)(L-2)}{2}\lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}}{(1-\lambda^2)^7}
\end{aligned} \tag{B.3}$$

$$\begin{aligned}
&g_3\left((L) \leftarrow \Gamma_4; \lambda\right)\\
&= \frac{4(2L+1)\lambda^L + 4(2L+1)\lambda^{L+1}}{(1-\lambda^2)^9}\\
&\quad + \frac{(\frac{1}{6}L^3 + L^2 - \frac{37}{6}L - 3)\lambda^L + 2(L-2)(2L+1)\lambda^{L+1} - \frac{(L-2)(L^2-16L-9)}{6}\lambda^{L+2}}{(1-\lambda^2)^8}\\
&\quad + \frac{\frac{L(L-1)(L-2)}{2}\lambda^{L+1} + \frac{(L+1)(L-1)(L-2)}{2}\lambda^{L+2} + \frac{L(L-1)(L-2)}{6}\lambda^{L+3}}{(1-\lambda^2)^7}
\end{aligned} \tag{B.4}$$

$$g_4\left((L) \leftarrow \Gamma_4; \lambda\right)$$

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

The generating function suitable for a symbolic interpretation in term of a generalized integrity basis are given in Table B1 for selected values of L.

Table B1. Expressions of the g_i Molien functions for four spatial vectors and selected (L) final irreducible representations.

i	Γ_{final}	$g_i\,(\Gamma_{\text{final}} \leftarrow \Gamma_4; \lambda)$
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	$\vdots$	

Appendix B.2. Generating function for five vectors

Let us write the five spatial vector generating function in the form,

$$g_1\left((L) \leftarrow \Gamma_5; \lambda\right) = \frac{\mathcal{N}_1\left((L) \leftarrow \Gamma_5; \lambda\right)}{\left(1-\lambda^2\right)^{12}}, \tag{B.6}$$

By coupling the generating function for one vector and the generating function for four vectors, the numerator is found to be:

$$\begin{aligned}
\mathcal{N}_1\left((L) \leftarrow \Gamma_5; \lambda\right) &= \frac{(L+4)(L+3)(L+2)(L+1)}{24}\lambda^{L} + \frac{(L+4)(L+3)(L+2)L}{6}\lambda^{L+1} \\
&+ \frac{(L+4)(L+3)(L+2)(L+1)}{8}\lambda^{L+2} - \frac{(L+4)(L+3)(L^2-3L-\frac{5}{2})}{3}\lambda^{L+3} \\
&- \frac{(L+4)(L+3)(L-3)(7L+2)}{12}\lambda^{L+4} - \frac{(L+4)(L-3)(2L+1)}{2}\lambda^{L+5} \\
&+ \frac{(L+4)(L-2)(L-3)(7L+5)}{12}\lambda^{L+6} + \frac{(L-2)(L-3)(L^2+5L+\frac{3}{2})}{3}\lambda^{L+7} \\
&- \frac{L(L-1)(L-2)(L-3)}{8}\lambda^{L+8} - \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+9} \\
&- \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+10}
\end{aligned} \tag{B.7}$$

The following six alternative forms of the generating function provide at least one expression with only positive coefficients for any L-values. In section 3.1, an algorithm to derive them will be explained.

$$\begin{aligned}
&g_2\left((L) \leftarrow \Gamma_5; \lambda\right) \\
&= \frac{\mathcal{N}_{2,1}\left((L) \leftarrow \Gamma_5; \lambda\right)}{\left(1-\lambda^2\right)^{12}} + \frac{\mathcal{N}_{2,2}\left((L) \leftarrow \Gamma_5; \lambda\right)}{\left(1-\lambda^2\right)^{11}} + \frac{\mathcal{N}_{2,3}\left((L) \leftarrow \Gamma_5; \lambda\right)}{\left(1-\lambda^2\right)^{10}} \\
&\quad + \frac{\mathcal{N}_{2,4}\left((L) \leftarrow \Gamma_5; \lambda\right)}{\left(1-\lambda^2\right)^{9}}
\end{aligned} \tag{B.8}$$

$$\begin{aligned}
&\mathcal{N}_{2,1}\left((L) \leftarrow \Gamma_5; \lambda\right) \\
&= \frac{(L+4)(L+3)(L+2)(L+1)}{24}\lambda^{L} + 20(2L+1)\lambda^{L+1} \\
&\quad + (-\frac{1}{24}L^4 - \frac{5}{12}L^3 - \frac{35}{24}L^2 + \frac{455}{12}L + 19)\lambda^{L+2} \\
&\mathcal{N}_{2,2}\left((L)\,; \Gamma_5; \lambda\right) \\
&= (\frac{1}{6}L^4 + \frac{3}{2}L^3 + \frac{13}{3}L^2 - 36L - 20)\lambda^{L+1} \\
&\quad - \frac{(L-3)(L^3+13L^2-406L-208)}{24}\lambda^{L+2} \\
&\quad - \frac{(L-3)(L^3+12L^2-58L-30)}{6}\lambda^{L+3} \\
&\mathcal{N}_{2,3}\left((L) \leftarrow \Gamma_5; \lambda\right) \\
&= -\frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^{L+2} - \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+3}
\end{aligned}$$

$$\begin{aligned}
&\mathcal{N}_{2,4}\left((L)\leftarrow\Gamma_5;\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_3\left((L)\,;\Gamma_5;\lambda\right)\\
&=\frac{\mathcal{N}_{3,1}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{12}}+\frac{\mathcal{N}_{3,2}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{11}}+\frac{\mathcal{N}_{3,3}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{10}}\\
&\quad+\frac{\mathcal{N}_{3,4}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{9}} \qquad \text{(B.9)}\\
&\mathcal{N}_{3,1}\left((L)\leftarrow\Gamma_5;\lambda\right)\\
&=\frac{(L+4)(L+3)(L+2)(L+1)}{24}\lambda^{L}+20(2L+1)\lambda^{L+1}\\
&\quad+(-\frac{1}{24}L^4-\frac{5}{12}L^3-\frac{35}{24}L^2+\frac{455}{12}L+19)\lambda^{L+2}\\
&\mathcal{N}_{3,2}\left((L)\leftarrow\Gamma_5;\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}\left((L)\leftarrow\Gamma_5;\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}\left((L)\leftarrow\Gamma_5;\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\left((L)\leftarrow\Gamma_5;\lambda\right)\\
&=\frac{\mathcal{N}_{4,1}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{12}}+\frac{\mathcal{N}_{4,2}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{11}}+\frac{\mathcal{N}_{4,3}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{10}}\\
&\quad+\frac{\mathcal{N}_{4,4}\left((L)\leftarrow\Gamma_5;\lambda\right)}{(1-\lambda^2)^{9}} \qquad \text{(B.10)}\\
&\mathcal{N}_{4,1}\left((L)\leftarrow\Gamma_5;\lambda\right)\\
&=20(2L+1)\lambda^{L}+20(2L+1)\lambda^{L+1}\\
&\mathcal{N}_{4,2}\left((L)\leftarrow\Gamma_5;\lambda\right)\\
&=(\frac{1}{24}L^4+\frac{5}{12}L^3+\frac{35}{24}L^2-\frac{455}{12}L-19)\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}_{4,3}\left((L)\,;\Gamma_5;\lambda\right)
\end{aligned}$$

$$= \frac{(L-3)(L^3+12L^2-58L-30)}{6}\lambda^{L+1} - \frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^{L+2}$$
$$- \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+3}$$

$$\mathcal{N}_{4,4}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2} + \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3}$$
$$+ \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4}$$

$$g_5\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= \frac{\mathcal{N}_{5,1}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{5,2}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{5,3}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{10}}$$
$$+ \frac{\mathcal{N}_{5,4}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{9}} \tag{B.11}$$

$$\mathcal{N}_{5,1}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= 20(2L+1)\lambda^L + 20(2L+1)\lambda^{L+1}$$

$$\mathcal{N}_{5,2}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= (\frac{1}{24}L^4 + \frac{5}{12}L^3 + \frac{35}{24}L^2 - \frac{455}{12}L - 19)\lambda^L + 5(2L+1)(2L-7)\lambda^{L+1}$$
$$- \frac{(L-3)(L^3+13L^2-406L-208)}{24}\lambda^{L+2}$$

$$\mathcal{N}_{5,3}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= (L-3)(2L-7)(2L+1)\lambda^{L+1} - \frac{(L-2)(L-3)(L^2-81L-40)}{24}\lambda^{L+2}$$

$$\mathcal{N}_{5,4}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= \frac{(L-2)(L-3)(L^2-10L-6)}{6}\lambda^{L+1} + \frac{L(L-1)(L-2)(L-3)}{4}\lambda^{L+2}$$
$$+ \frac{(L+1)(L-1)(L-2)(L-3)}{6}\lambda^{L+3} + \frac{L(L-1)(L-2)(L-3)}{24}\lambda^{L+4}$$

$$g_6\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= \frac{\mathcal{N}_{6,1}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{12}} + \frac{\mathcal{N}_{6,2}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{11}} + \frac{\mathcal{N}_{6,3}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{10}}$$
$$+ \frac{\mathcal{N}_{6,4}\left((L) \leftarrow \Gamma_5;\lambda\right)}{(1-\lambda^2)^{9}} \tag{B.12}$$

$$\mathcal{N}_{6,1}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= 20(2L+1)\lambda^L + 20(2L+1)\lambda^{L+1}$$

$$\mathcal{N}_{6,2}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= 5(2L+1)(2L-9)\lambda^L + 5(2L+1)(2L-7)\lambda^{L+1}$$

$$\mathcal{N}_{6,3}\left((L) \leftarrow \Gamma_5;\lambda\right)$$
$$= \frac{(L-3)(L^3+13L^2-406L-208)}{24}\lambda^L + (L-3)(2L+1)(2L-7)\lambda^{L+1}$$

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

The generating function suitable for a symbolic interpretation in term of a generalized integrity basis are given in Table B2 for selected values of L.

Table B2. Expressions of the g_i Molien functions for five spatial vectors and selected (L) final irreducible representations.

i	Γ_{final}	$g_i\,(\Gamma_{\mathrm{final}} \leftarrow \Gamma_5;\lambda)$
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	⋮	⋮