

Molien series and low-degree invariants for a natural action of $\mathrm{SO}(3) \wr \mathbb{Z}_2$

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1. Introduction and motivation

Associated to any pair of representations D_1, D_2 of finite or compact Lie groups $\mathbf{G}_1, \mathbf{G}_2$ on finite-dimensional complex linear spaces V_1, V_2 respectively there is a natural action (representation) $D_1 \otimes D_2$ of $\mathbf{G}_1 \times \mathbf{G}_2$ on the tensor product $V_1 \otimes V_2$ determined by

$$D_1 \otimes D_2(g_1, g_2): v_1 \otimes v_2 \mapsto D_1(g_1)v_1 \otimes D_2(g_2)v_2. \quad (1)$$

If D_1, D_2 are irreducible then $D_1 \otimes D_2$ is irreducible, and indeed every irreducible representation of $\mathbf{G}_1 \times \mathbf{G}_2$ is of this form [1, II (4.14)]. The space $V_1 \otimes V_2$ can be identified with the space $L(V_2^*, V_1)$ of linear maps from V_2^* to V_1 by

$$v_1 \otimes v_2: V_2^* \rightarrow V_1: \alpha \mapsto \alpha(v_2)v_1 \quad (2)$$

and the representation $D_1 \otimes D_2$ corresponds to the action on $L(V_2^*, V_1)$ by left and right multiplication:

$$D_1 \otimes D_2(g_1, g_2): A \mapsto D_1(g_1)A D_2(g_2)^* \quad (3)$$

for all $A \in L(V_2^*, V_1)$, where $*$ denotes the dual object (space or linear map).

$$\begin{array}{ccc} V_2^* & \xrightarrow{A} & V_1 \\ D_2(g_2)^* \uparrow & & \downarrow D_1(g_1) \\ V_2^* & \xrightarrow{D_1 \otimes D_2(g_1, g_2)A} & V_1 \end{array}$$

If V_2 has an inner product and it is assumed (as may always be done) that D_2 acts by unitary transformations, then V_2^* is identified with V_2 and $D_2(g_2)^*$ becomes the complex conjugate transposition of $D_2(g_2)$.

1.1. Wreath product actions

In the particular case where $V_1 = V_2 = V$, $\mathbf{G}_1 = \mathbf{G}_2 = \mathbf{G}$ and $D_1 = D_2 = D$ then there is an extra symmetry inherent in the situation, namely the \mathbb{Z}_2 -action of $*$ on $L(V^*, V)$. Combined with $D \otimes D$ this gives an action \widetilde{D} of the *wreath product*

$$\Gamma := \mathbf{G} \wr \mathbb{Z}_2 \cong (\mathbf{G} \times \mathbf{G}) \rtimes \mathbb{Z}_2 \quad (4)$$

on $L(V^*, V)$. Explicitly, each element of Γ can be written uniquely in the form $(g, h)\tau^\varepsilon$ with $\varepsilon \in \{0, 1\}$ where $h \in \mathbf{G}$ and τ generates \mathbb{Z}_2 . Those elements with $\varepsilon = 0$ form a subgroup $\Gamma_0 < \Gamma$ of index 2 isomorphic to $\mathbf{G} \times \mathbf{G}$. Elements of Γ_0 act on $L(V^*, V)$ by

$$\widetilde{D}(g, h): A \mapsto D(g)A D(h)^* \quad (5)$$

while the elements of the other coset Γ_1 act by

$$\widetilde{D}(g, h)\tau: A \mapsto D(g)A^* D(h)^*. \quad (6)$$

In this paper we focus on the case when $\mathbf{G} = \mathrm{SO}(3)$, and are interested in studying real-valued *invariants* for real wreath product actions as just described.

1.2. Physical motivation

It is well known [1, 2] that the irreducible representations of $\mathbf{SO}(3)$ are each characterized by a nonnegative integer ℓ , with (up to isomorphism) precisely one such representation $D^{(\ell)}$ for each given ℓ on a linear space $V^{(\ell)}$ of dimension $2\ell + 1$. Group actions of the wreath product type involving $\mathbf{SO}(3)$ arise in certain physical applications such as the study of rotating ellipsoids [3] (where $\ell = 1$) or phase transitions of biaxial nematic liquid crystals [4] (where $\ell = 2$), as well as for other groups in coupled cell networks [5].

In the liquid crystal setting the average orientation of the molecules is traditionally described by assigning an orientational single particle probability density function $f(\Omega)$, where $\Omega \in \mathbf{SO}(3)$ is the molecular orientation with respect to the laboratory frame. The function f is then usually expanded into Fourier components given by the matrix entries of $D^{(\ell)}$, which constitute a natural orthonormal basis in this context. The coefficients of this expansion are identified with the order parameters, i.e., those scalars able to describe the phase of the system and the transition from a phase to another. In general there are an infinite number of order parameters; for practical convenience, however, the expansion is usually truncated at the second-rank level ($\ell = 2$) and only second-rank order parameters are used to study the system. See [6] for careful discussion of these issues.

The order parameters and the invariants built upon them play a key role in the study of phase transitions in that they allow the construction of Landau-like free energy for the system. A general strategy to derive a Landau free-energy density from a molecular field theory, which also applies to biaxial nematic liquid crystals, is formulated in [7, 8]. In this case, the orientational probability function, truncated at $\ell = 2$, turns out to be a family of Maxwell–Boltzmann distributions of the form

$$f(\eta, \Omega) = \text{const.} \times \exp(\eta \cdot D(\Omega)), \quad (7)$$

where D is a representation of $\mathbf{SO}(3)$ on a space $V \cong \mathbf{R}^n$ of orientational order parameters Q ; sometimes $D(\Omega)$ is written as $Q(\Omega)$ [8]. Here $\eta \in L(V, V)$ plays the role of a set of Lagrange multipliers and the dot denotes the inner product $A \cdot B = \text{trace}(A^T B)$ on $L(V, V)$. The entropy difference function $\Delta S: L(V, V) \rightarrow \mathbf{R}$ given by

$$\Delta S(\eta) = -k \int_{\mathbf{SO}(3)} f(\eta, \Omega) \ln f(\eta, \Omega) d\Omega \quad (8)$$

plays a central part in the study of phase transitions [6] and is invariant under the action of $\mathbf{SO}(3)$ on $L(V^*, V)$ associated to D , after V^* is identified with V by the usual inner product on \mathbf{R}^n : this can be seen from the properties of the inner product and the fact that

integrating over $R \in \mathbf{SO}(3)$ is the same as integrating over $R_0 R$ (for fixed $R_0 \in \mathbf{SO}(3)$) or over $R^T = R^{-1}$. See [4] for further details.

Usually the molecular and the phase symmetries are assumed at the beginning of these calculations, with the advantage of greatly simplifying all the subsequent algebra. The drawback, however, is that when a molecule with a different symmetry is considered, the previous derivations must be performed again from the beginning. More importantly, general considerations on the structure of the theory, i.e., what are the phase transitions allowed by the theory at $\ell = 2$ and what is their nature (first or second order), are difficult to obtain. It is therefore of interest to study the general structure of the entropy invariants independently of the symmetry of the molecules and the phases at hand and subsequently to make the simplifications induced by the molecular and phase symmetry.

1.3. The ring of invariant functions

An *invariant function* (or simply *invariant*) for a representation D of a group \mathbf{G} on a real (respectively complex) linear space V is a function $f: V \rightarrow \mathbf{R}$ (respectively \mathbf{C}) such that $f \circ D(g) = f$ for all $g \in \mathbf{G}$. Sums and products of invariants are also invariants, and the set of invariants for D forms a ring, as does the set of C^r invariants for $0 \leq r \leq \infty$ (or ω) and the set of polynomial invariants. If \mathbf{G} is a finite group or reductive linear algebraic group [9] the ring \mathcal{R} of polynomial invariants has a finite set of algebraic generators (integrity basis) with additional structure: the polynomial invariants form a *free module* over a subring $\mathcal{R}_1 \subset \mathcal{R}$ [10]. Explicitly this means that there is a set $\{f_1, \dots, f_r\}$ of *algebraically independent* polynomial generators for \mathcal{R}_1 and a set $\{h_1, \dots, h_k\}$ of *linearly independent* invariant polynomials in \mathcal{R} with the property that every polynomial invariant f can be expressed uniquely in the form

$$f = \sum_{j=1}^k h_j p_j,$$

where the $p_j \in \mathcal{R}_1$, that is to say p_j is a polynomial in $\{f_1, \dots, f_r\}$. The $\{f_i\}$ and $\{h_j\}$ are often called *primary* and *secondary* generators respectively.

As an example, for the case of $\mathbf{G} = \mathbf{Z}_2$ acting on \mathbf{R}^2 by $(x, y) \mapsto (-x, -y)$ we have $k = r = 2$ with $\{h_1, h_2\} = \{1, xy\}$ and $\{f_1, f_2\} = \{x^2, y^2\}$, since every invariant polynomial can be written uniquely as $p_1 + xy p_2$ with p_1, p_2 polynomials in $\{x^2, y^2\}$.

To display the algebraic structure of the ring of invariant functions for group actions of this kind may be feasible (although complicated) for groups and representations of low dimension, as has been carried out for example in [11] for a related representation of $\mathbf{G} = \mathbf{GL}(2)$. It is totally impractical in our case where $\mathbf{I} = \mathbf{SO}(3) \wr \mathbf{Z}_2$ acts on the 25-dimensional space $L(V^*, V)$ with $\dim V = 5$, but we are nevertheless able to derive the corresponding *Molien series* both for the subgroup $\mathbf{I}_0 \cong \mathbf{SO}(3) \times \mathbf{SO}(3)$ and for the full group \mathbf{I} . For a given representation D of a group \mathbf{G} this formal power series $\mathcal{P}_D(t)$ (or $\mathcal{P}_G(t)$ if D is understood) has the property that the coefficient of t^m is a non-negative integer equal to the dimension of the linear space of D -invariant polynomials of homogeneous degree m : see [12, 13] for example. The Molien series is obtained in the form of a rational function from which we deduce that there are 19 primary invariants (to be expected, since $\dim \mathbf{I} = 6$) and at least 363 481 512 secondary invariants. We are able to give explicit generators at degrees 2, 3 and 4 and in doing so we uncover some unexpected algebraic properties of tensor contractions that yield these generators.

1.4. Quaternions, $\mathbf{SO}(4)$ and $\mathbf{SO}(3) \times \mathbf{SO}(3)$

The group $\mathbf{SU}(2)$ is isomorphic to the group \mathbf{Q}^* of unit quaternions, and acts orthogonally on the space $\mathbf{Q} \cong \mathbf{R}^4$ of all quaternions by

$$q: x \mapsto qh(x)\bar{q}, \tag{9}$$

where we identify $x = (x_0, x_1, x_2, x_3)^T \in \mathbf{R}^4$ with

$$h(x) = x_0 + x_1 i + x_2 j + x_3 k \in \mathbf{Q}. \tag{10}$$

This action leaves the real subspace invariant and so induces an action on its orthogonal complement (pure quaternions) $\cong \mathbf{R}^3$, which defines a projection

$$\pi: \mathbf{SU}(2) \rightarrow \mathbf{SO}(3). \quad (11)$$

It is straightforward to check that the kernel of π is $\{E, -E\}$ where E denotes the identity matrix in $\mathbf{SU}(2)$, so that the group $\mathbf{SU}(2)$ is a double cover of $\mathbf{SO}(3)$. Thus every representation of $\mathbf{SO}(3)$ induces one of $\mathbf{SU}(2)$, while the converse is true only if $-E$ acts trivially.

The irreducible complex representations of $\mathbf{SU}(2)$ can be explicitly constructed on complex homogeneous polynomials in two variables of degree $d \geq 0$ (see e.g. [1 II (5.3)]). Since the space of such polynomials has complex dimension $d + 1$, we have such a representation for each positive integer dimension, and clearly the element $-E$ acts trivially if and only if d is even. Thus it is the odd-dimensional irreducible (complex) representations of $\mathbf{SU}(2)$ that give rise to the irreducible complex representations of $\mathbf{SO}(3)$ which, since these are of real type [1, II 6], correspond to representations in each odd (real) dimension $2\ell + 1$. With this convention, the even-dimensional irreducible complex representations of $\mathbf{SU}(2)$ can be labelled by non-integer values of ℓ which we call *half-integers*.

Let

$$\text{Spin}_4 = \mathbf{Q}^* \times \mathbf{Q}^*. \quad (12)$$

There is a natural action of Spin_4 on \mathbf{Q} given by

$$(q_1, q_2): q \mapsto q_1 q \bar{q}_2. \quad (13)$$

Viewed as an action on \mathbf{R}^4 , this is orthogonal and has determinant 1, and thus defines a homomorphism

$$\tilde{\pi}: \text{Spin}_4 \rightarrow \mathbf{SO}(4). \quad (14)$$

The kernel is again \mathbf{Z}_2 , here generated by $(-E, -E)$ and so we have an isomorphism

$$\text{Spin}_4 / \mathbf{Z}_2 = \mathbf{Q}^* \times \mathbf{Q}^* / \mathbf{Z}_2 \rightarrow \mathbf{SO}(4). \quad (15)$$

At the same time we have an isomorphism

$$\mathbf{SU}(2) \times \mathbf{SU}(2) / \mathbf{Z}_2 \times \mathbf{Z}_2 \rightarrow \mathbf{SO}(3) \times \mathbf{SO}(3), \quad (16)$$

and so it is natural to ask: when does an (ℓ_1, ℓ_2) representation of $\mathbf{SU}(2) \times \mathbf{SU}(2)$ correspond to a representation of $\mathbf{SO}(4)$? This is the case if and only if both numbers ℓ_1, ℓ_2 are half-integers or both are integers, since $(-E, -E)$ must act trivially and therefore $-E$ must act in the same way (change the sign or not change the sign) in both factors. To summarize:

Proposition 1. *The tensor product of two (complex) irreducible representations of $\mathbf{SU}(2)$ with labels ℓ_1, ℓ_2 projects to a representation of $\mathbf{SO}(4)$ (of dimension $(2\ell_1 + 1)(2\ell_2 + 1)$) if and only if $\ell_1 + \ell_2$ is an integer. In particular, the tensor product of two (complex, real) irreducible representations of $\mathbf{SO}(3)$ always projects to a representation of $\mathbf{SO}(4)$.*

In table 1 we list the labels for irreducible representations of $\mathbf{SU}(2) \times \mathbf{SU}(2)$ for dimensions $(2\ell_1 + 1)(2\ell_2 + 1)$ up to 35. Observe that in the cases where $\ell_1 \neq \ell_2$ we have in addition to the given pair, the pair (ℓ_2, ℓ_1) . Our interest in this paper is in the cases where (ℓ_1, ℓ_2) are positive integers, and $\ell_1 = \ell_2 = \ell$ so that conjugate transposition also acts on the tensor product representation. For practical purposes this restricts us to $\ell = 1$ or $\ell = 2$. For further detailed information on subgroups of $\mathbf{SO}(4)$, quaternions and rotations see [14, 15].

Table 1. Labels for irreducible representations of $\mathbf{SU}(2) \times \mathbf{SU}(2)$ for dimensions $(2\ell_1 + 1)(2\ell_2 + 1)$ up to 35.

dim	(ℓ_1, ℓ_2)	dim	(ℓ_1, ℓ_2)
1	(0, 0)	19	(0, 9)
3	(0, 1)	20	$(\frac{1}{2}, \frac{9}{2})$
4	$(\frac{1}{2}, \frac{1}{2})$	21	(0, 10), (1, 3)
5	(0, 2)	23	(0, 11)
7	(0, 3)	24	$(\frac{1}{2}, \frac{11}{2}), (\frac{3}{2}, \frac{5}{2})$
8	$(\frac{1}{2}, \frac{3}{2})$	25	(0, 12), (2, 2)
9	(0, 4), (1, 1)	27	(0, 13), (1, 4)
11	(0, 5)	28	$(\frac{1}{2}, \frac{13}{2})$
12	$(\frac{1}{2}, \frac{5}{2})$	29	(0, 14)
13	(0, 6)	31	(0, 15)
15	(0, 7), (1, 2)	32	$(\frac{1}{2}, \frac{15}{2}), (\frac{3}{2}, \frac{7}{2})$
16	$(\frac{1}{2}, \frac{7}{2}), (\frac{3}{2}, \frac{3}{2})$	33	(0, 16), (1, 5)
17	(0, 8)	35	(0, 17), (2, 3)

2. Molien functions

Associated to any n -dimensional (real or complex) representation D of a compact Lie group \mathbf{H} is its *Molien integral*

$$\int_{\mathbf{H}} \det(I - tD(h))^{-1} dh \quad (17)$$

with respect to the normalized (Haar) invariant measure on \mathbf{H} . The integral is a *sum* if \mathbf{H} is finite. As shown by Molien in 1897, for finite groups this integral has the remarkable property that its formal expansion as a power series in t is precisely the Molien series $\mathcal{P}_{\mathbf{H}}(t)$. The result holds also for compact Lie groups [22]. Moreover, when appropriately expressed as a rational function of t , the Molien series conveys further information on the structure of the ring of invariants: see e.g. [12, 13]. To be more precise, if \mathbf{H} is a group as in section 1.3, which applies in our case, and there are r primary invariants of homogeneous degrees d_1, \dots, d_r then the Molien series is the Taylor series at $t = 0$ of a rational function $P(t)/Q(t)$ with

$$Q(t) = \prod_{i=1}^r (1 - t^{d_i}) \quad (18)$$

and such that the coefficient of t^m in $P(t)$ is the number of linearly independent secondary generators h_j with degree m . For example, in the case $\mathbf{H} = \mathbf{Z}_2$ in section 1.3 we see that

$$\begin{aligned} \mathcal{P}_{\mathbf{H}}(t) &= \frac{1}{2} \left((1 - t)^{-2} + (1 + t)^{-2} \right) \\ &= (1 + t^2) (1 - t^2)^{-2} \end{aligned} \quad (19)$$

consistent with two primary generators of degree 2 and one non-constant secondary generator also of degree 2.

Unfortunately, an expression of $\mathcal{P}_{\mathbf{H}}(t)$ as a rational function $P(t)/Q(t)$ of the above form does not guarantee its interpretation in terms of primary and secondary generators, as may be seen for example by multiplying both $P(t)$ and $Q(t)$ by $(1 + t^{d_1})$. It might be expected that the true algebraic picture is represented by $P(t)/Q(t)$ in ‘simplest’ form, but even this is not the case: an example with $\mathbf{H} = \mathbf{Z}_2 \times \mathbf{Z}_4$ is given in [16]. We shall therefore need to consider the expression of $\mathcal{P}_{\mathbf{D}}(t)$ as a rational function in more than one way.

Definition 1. Let $\mathcal{P}_{\mathbf{D}}(t)$ be a Molien series expressed as a rational function $P(t)/Q(t)$ such that the $Q(t)$ is a product of terms of the form $(1 - t^{d_i})$ while $P(t)$ has only nonnegative coefficients. We call $P(t)/Q(t)$ an *admissible rational expression* of the series $\mathcal{P}_{\mathbf{D}}(t)$.

2.1. The Molien integrand

Since $\det(I - tD(g)) = t^n \det(t^{-1}I - D(g))$ the integrand in (17) can always be expressed in terms of the eigenvalues of $D(g)$ when these are known. In the case of a unitary representation the Molien series is automatically real.

We shall apply this to the case of $\mathbf{H} = \mathbf{F} = \mathbf{G} \wr \mathbf{Z}_2$ acting on $L(V^*, V)$ via \tilde{D} associated to an action D of \mathbf{G} on V as in section 1.1. First, we extend the action of \mathbf{G} to its associated action on the complex linear space $V \otimes \mathbf{C}$ in order to be able to use a basis of (complex) eigenvectors for each element of $D(\mathbf{G})$. For $g \in \mathbf{G}$ let $\Lambda(g) \subset \mathbf{C}$ denote the corresponding set of eigenvalues $\{\lambda_1, \dots, \lambda_n\}$ of $D(g)$ (with repeats) where $\dim V = n$.

Proposition 2. Let $(M, N) \in \Gamma_0 \cong \mathbf{G} \times \mathbf{G}$.

- (i) The eigenvalues ν of $\tilde{D}(g, h)$ are given by $\nu = \lambda_i \bar{\mu}_j$ where $\lambda_i, \mu_j \in \Lambda(g), \Lambda(h)$ respectively.
- (ii) The eigenvalues γ of $\tilde{D}((g, h)\tau)$ are given by $\gamma^2 = \bar{\beta}_i \bar{\beta}_j$ and by $\gamma = \bar{\beta}_i$ where $\beta_i, \beta_j \in \Lambda(gh)$.

Proof. For simplicity we take D as understood and drop it from the notation.

- (i) If $\{u_i\}, \{v_j\}$ are (complex) eigenbases for g, h respectively ($i, j = 1, \dots, n$) then the n^2 matrices $\{u_i v_j^*\}$ clearly form an eigenbasis for (g, h) with eigenvalues ν as stated.
- (ii) First note that the eigenvalues of gh coincide with those of hg since w is an eigenvector of gh if and only if hw is an eigenvector of hg with the same eigenvalue. Next, let u, v be (complex) eigenvectors of hg with distinct eigenvalues λ, μ respectively. Write $\tilde{u} = gu$ and $\tilde{v} = gv$, so that $h\tilde{u} = \lambda u$ and $h\tilde{v} = \mu v$. We then see that

$$(g, h)\tau(\tilde{u}v^*) = g\tilde{u}v^*h^* = \bar{\lambda}\tilde{v}u^* \quad (20)$$

and

$$(g, h)\tau(\tilde{v}u^*) = g\tilde{v}u^*h^* = \bar{\mu}\tilde{u}v^*. \quad (21)$$

Therefore the two-dimensional subspace $\text{span}\{\tilde{u}v^*, \tilde{v}u^*\}$ of $L(V \otimes \mathbf{C})$ is invariant under $(g, h)\tau$, and with respect to the basis $\{\tilde{u}v^*, \tilde{v}u^*\}$ the matrix of $(g, h)\tau$ is

$$\begin{pmatrix} 0 & \bar{\mu} \\ \bar{\lambda} & 0 \end{pmatrix}, \quad (22)$$

whose eigenvalues γ satisfy $\gamma^2 = \bar{\lambda}\bar{\mu}$ as claimed. We observe also that $\tilde{u}u^*$ is an eigenvector of $(g, h)\tau$ with eigenvalue $\bar{\lambda}$.

We apply this now to the case of $\mathbf{G} = \mathbf{SO}(3)$ acting on $V = V^{(\ell)}$ by the $D^{(\ell)}$ representation where $\ell = 1, 2$. The case $\ell = 1$ is straightforward and doubtless well known in the invariant theory literature, but we include it here as illustration of the methods employed in the considerably more complicated $\ell = 2$ case. Using proposition 2 it is straightforward to write down the Molien integrand in (17). The eigenvalues of $M \in \mathbf{SO}(3)$ are $\{1, e^{i\theta}, e^{-i\theta}\}$ for some θ which we call the *rotation angle*. Let $N \in \mathbf{SO}(3)$ with rotation angle ϕ , and suppose MN has rotation angle ψ . Write (with new notation) $z = e^{i\theta}$, $w = e^{i\phi}$ and $v = e^{i\psi}$.

2.2. The case $\ell = 1$

The eigenvalues of $D^{(1)}(M)$, $D^{(1)}(N)$ are those of M , N and so by proposition 2 the eigenvalues of $\tilde{D}^{(1)}(M, N)$ are

$$\{z^j w^k\} = \{e^{i(j\theta + k\phi)}\}, \quad j, k \in \{-1, 0, 1\} \quad (23)$$

while the eigenvalues of $\tilde{D}^{(1)}((M, N)\tau)$ are

$$\{1, 1, -1, e^{i\psi}, e^{-i\psi}, \pm e^{i\psi/2}, \pm e^{-i\psi/2}\}. \quad (24)$$

Therefore for $g = (M, N) \in \mathbf{I}_0$ we have

$$\det(I - t\tilde{D}^{(1)}(g)) = \prod_{j=-1}^1 \prod_{k=-1}^1 (1 - tz^j w^k), \quad (25)$$

while for $g = (M, N)\tau \in \mathbf{I}_1$ we have

$$\det(I - t\tilde{D}^{(1)}(g)) = (1 - t)^2(1 + t)(1 - tv)(1 - t\bar{v})(1 - t^2v)(1 - t^2\bar{v}). \quad (26)$$

2.3. The case $\ell = 2$

The eigenvalues of $D^{(2)}(M)$ are $\{1, e^{i\theta}, e^{-i\theta}, e^{2i\theta}, e^{-2i\theta}\}$ and so the eigenvalues of $\tilde{D}^{(2)}(M, N)$ are

$$\{z^j w^k\} = \{e^{i(j\theta + k\phi)}\}, \quad j, k \in \{-2, -1, 0, 1, 2\}, \quad (27)$$

while the eigenvalues of $\tilde{D}^{(2)}((M, N)\tau)$ are

1	three times
-1	twice
$\pm e^{\pm i\psi/2}$	twice each
$e^{\pm i\psi}$	twice each
$-e^{\pm i\psi}$	once each
$e^{\pm 2i\psi}$	once each
$\pm e^{\pm 3i\psi/2}$	once each

(a total of 25 eigenvalues). Therefore for $g \in \Gamma_0$

$$\det\left(I - t\tilde{D}^{(2)}(g)\right) = \prod_{j=-2}^2 \prod_{k=-2}^2 (1 - tz^j w^k), \quad (28)$$

while for $g \in \Gamma_1$ the expression becomes

$$\begin{aligned} \det\left(I - t\tilde{D}^{(2)}(g)\right) &= (1-t)^3(1+t)^2(1-t^2v)^2(1-t^2\bar{v})^2(1-tv)^2(1-t\bar{v})^2 \\ &\quad \times (1+tv)(1+t\bar{v})(1-tv^2)(1-t\bar{v}^2)(1-t^2v^3)(1-t^2\bar{v}^3). \end{aligned} \quad (29)$$

2.4. Evaluation of the Molien integrals

When the integration (17) is carried out over the Lie group $\Gamma = \mathbf{G} \wr \mathbf{Z}_2$ the result is half of the sum of integrals over the subgroup Γ_0 and the coset Γ_1 :

$$\int_{\Gamma} = \frac{1}{2} \left(\int_{\Gamma_0} + \int_{\Gamma_1} \right) \quad (30)$$

since the normalized Haar measure for Γ when restricted to Γ_0 is half the Haar measure of Γ_0 . As described in [1, IV(1.11)] for example, the Weyl integral formula shows that an integral over a compact Lie group can be decomposed into a double integral over a maximal torus and over the quotient of the group by this torus. In the case when the integrand is a class function (invariant under conjugation in the group) then the latter integral becomes trivial, and the total integral reduces to an integral over the maximal torus at the cost of introducing a further term into the integrand that we call the *Weyl factor*, and dividing by the order $|W|$ of the *Weyl group* W . The integral over the maximal torus is expressed in terms of angular variables and is evaluated using residue calculus. Since the aim is to find $\mathcal{P}_{\Gamma}(t)$ as an infinite series in t we can regard t as a small real variable and in any case with $|t| < 1$, and this restriction can be usefully exploited when evaluating residues.

For the case of $\mathbf{G} = \mathbf{SO}(3)$ with which we are concerned, a maximal torus (circle) in \mathbf{G} is given by the matrices

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix} \quad (31)$$

for $0 \leq \theta < 2\pi$, and integration is over the unit circle regarded as the circle $|z| = 1$ in the complex plane. The Weyl factor can be found to be

$$(1-z)(1-\bar{z}) = 2(1-\cos \theta) \quad (32)$$

(see [17, 18]) while $W = \mathbf{Z}_2$ so $|W| = 2$ and therefore the Molien integral (17) for the $\tilde{D}^{(\ell)}$ representation of Γ_0 becomes

$$\mathcal{P}_{\Gamma_0}^{\ell}(t) = -\frac{1}{16\pi^2} \int_{|z|=1} \int_{|w|=1} \frac{(1-z)^2(1-w)^2}{\prod_{j,k=-\ell}^{\ell} (1-tz^j w^k)} \frac{dz}{z^2} \frac{dw}{w^2} \quad (33)$$

for $\ell = 1$ or $\ell = 2$, with $4\pi^2$ the normalising factor of the invariant measure on the maximal torus $S^1 \times S^1$ of Γ_0 .

For the second coset Γ_1 of Γ in the case $\ell = 1$ we have from (26) (with slight abuse of notation as Γ_1 is not a group)

$$\begin{aligned} \mathcal{P}_{I_1}^1(t) &= \frac{1}{4\pi i} (1-t)^{-2} (1+t)^{-1} \\ &\times \int_{|v|=1} \frac{(1-v)(1-v^{-1})}{(1-tv)(1-tv^{-1})(1-t^2v)(1-t^2v^{-1})} \frac{dv}{v}, \end{aligned} \quad (34)$$

whereas for $\ell = 2$ we have the slightly more complicated expression

$$\mathcal{P}_{I_1}^2(t) = \frac{1}{4\pi i} (1-t)^{-3} (1+t)^{-2} \int_{|v|=1} \frac{(1-v)(1-v^{-1})}{K(v, t)} \frac{dv}{v}, \quad (35)$$

where from (29)

$$\begin{aligned} K(v, t) &= (1-tv)^2 (1-t\bar{v})^2 (1+tv)(1+t\bar{v}) (1-tv^2)(1-t\bar{v}^2) \\ &\times (1-t^2v)^2 (1-t^2\bar{v})^2 (1-t^2v^3)(1-t^2\bar{v}^3) \\ &= v^{-10} (1-tv)(1-tv^2)(1-t^2v)^2 (1-t^2v^2)(1-t^2v^3) \\ &\times (v-t)(v^2-t)(v^2-t^2)(v-t^2)^2 (v^3-t^2). \end{aligned} \quad (36)$$

Note that for I_1 the calculation of the Molien integral (17) reduces to a single integral since by (29) the expression $\det[I - t\bar{D}((M, N)\tau)]$ depends only on the rotation angle ψ of the product MN . More precisely, if $f(M, N) = \tilde{f}(L)$ with $L = MN$ then

$$\int_{\mathbf{G} \times \mathbf{G}} f(M, N) d(M, N) = \int_{\mathbf{G}} dN \int_{\mathbf{G}} \tilde{f}(MN) dM = \int_{\mathbf{G}} \tilde{f}(L) dL, \quad (37)$$

where we have used the facts that the measure is normalized and \mathbf{G} -invariant.

2.5. Integration in the case $\ell = 1$

Since $|w| = 1$ and $|t| < 1$ the only terms in the denominator that give rise to nonzero residues in the z -integral in $\mathcal{P}_{I_0}^1(t)$ are those with $j = -1$, that is $z = tw^k$ for $k = -1, 0, 1$, as well as $z = 0$. Thus

$$\mathcal{P}_{I_0}^1(t) = \frac{1}{8\pi i} \int_{|w|=1} (R_{-1}(w) + R_0(w) + R_1(w)) dw, \quad (38)$$

where $R_k(w)$ denotes the residue at $z = tw^k$ of the function $K(w)F_1(z, w)$ where

$$K(w) = \frac{(1-w)^2 w^{-2}}{(1-tw^{-1})(1-t)(1-tw)} \quad (39)$$

and

$$F_1(z, w) := \frac{(1-z)^2 z^{-2}}{(1-tz^{-1}w^{-1})(1-tz^{-1})(1-tz^{-1}w)(1-tzw^{-1})(1-tz)(1-tzw)} \quad (40)$$

as it is easy to verify that the residue at $z = 0$ is zero. It is straightforward (although a little tedious and best automated) to calculate that $R_k(w) = wS_k(w)^{-1}$ ($k = -1, 0, 1$) where

$$S_{-1}(w) = t(t+1)(1-t)^2(w+1)(tw-1)(t^2-w)(w+t) \quad (41)$$

$$S_0(w) = t(t+1)(w-t^2)(w-t)(1-tw)(t^2w-1) \quad (42)$$

$$S_1(w) = t(t+1)(1-t)^2(w+1)(tw+1)(1-t^2w)(w-t). \quad (43)$$

We thus see that the residues of (38) inside the unit circle occur where $w = \pm t, t^2$ and further calculation gives that

$$\mathcal{P}_{I_0}^1(t) = \left((1-t)^3(t^2+1)(t^2+t+1)(t+1)^2 \right)^{-1} = \left((1-t^2)(1-t^3)(1-t^4) \right)^{-1} \quad (44)$$

which when expanded as a power series in t gives

$$\begin{aligned} \mathcal{P}_{I_0}^1(t) &= 1 + t^2 + t^3 + 2t^4 + t^5 + 3t^6 + 2t^7 + 4t^8 \\ &\quad + 3t^9 + 5t^{10} + 4t^{11} + 7t^{12} + O(t^{13}). \end{aligned} \quad (45)$$

However, the series (45) is less informative than the rational function expression (44) which suggests that there are three primary invariants of degrees 2, 3, 4 and no secondary invariants. In fact primary invariants are

$$\text{tr}(A^T A), \quad \det(A), \quad \text{tr}(A^T A A^T A). \quad (46)$$

Since by the Cayley–Hamilton theorem every 3×3 matrix B satisfies its characteristic equation

$$B^3 - \text{tr}(B)B^2 + \frac{1}{2}(\text{tr}(B)^2 - \text{tr}(B^2))B + \det(B)I = 0, \quad (47)$$

applying this to $B = A^T A$ shows how ‘natural’ invariants of higher degree such as $\text{tr}(A^T A A^T A A^T A)$ may be expressed in terms of the primary generators (46).

The integral (34) for $\mathcal{P}_{I_1}^1(t)$ is simpler to evaluate. The residues inside the unit circle are given by $v = t, t^2$ with a zero residue at $v = 0$, and we find

$$\mathcal{P}_{I_1}^1(t) = \left((1-t^2)(1-t^3)(1-t^4) \right)^{-1} \quad (48)$$

which, remarkably, is the same as $\mathcal{P}_{I_0}^1(t)$. How can the Molien series

$$\mathcal{P}_I^1(t) = \frac{1}{2}(\mathcal{P}_{I_0}^1(t) + \mathcal{P}_{I_1}^1(t)) \quad (49)$$

be the same as that of the proper subgroup I_0 ? This apparent anomaly is resolved by the observation in [3] that polar decomposition (every matrix can be written as the product of an orthogonal and a symmetric matrix) implies that A^T lies on the same I_0 -orbit as A , and so every invariant for I_0 is an invariant for τ and hence for $I_0 \cup I_1$. This simplification does not occur in the case $\ell = 2$, however, because not every element of $\mathbf{SO}(5)$ is of the form $D^{(2)}(M)$ with $M \in \mathbf{SO}(3)$.

2.6. Integration in the case $\ell = 2$

The calculations here become considerably more complicated, and hardly feasible to carry out by hand. We have used MAPLE to assist with the residue calculations and the subsequent algebra.

2.6.1. Residues of the z -singularities. The terms in the denominator of the integrand (33) for $\mathcal{P}_{I_0}^2(t)$ that contribute to residues for the z -integral are those with $j = -1, -2$. For

$k = -2, \dots, 2$ we write $R_{1,k}(w, t)$ to denote the z -residue that occurs at $z = tw^k$ and $R_{2,k}(w, t)$ for the sum of the residues that occur at $z = \pm \sqrt{tw^k}$. We obtain the following results, most conveniently expressed in terms of the *inverses* of the $R_{n,k}$ for $n = 1, 2$:

$\boxed{n=1}$

$$-w^{29}t^4R_{1,-2}^{-1} = T_{1,-2}(w, t)Q_{1,-2}(w, t), \quad (50)$$

$$-w^{17}t^4R_{1,-1}^{-1} = T_{1,-1}(w, t)Q_{1,-1}(w, t), \quad (51)$$

$$-w^{13}t^4R_{1,0}^{-1} = T_{1,0}(w, t)Q_{1,0}(w, t), \quad (52)$$

$$-w^{17}t^4R_{1,1}^{-1} = T_{1,1}(w, t)Q_{1,1}(w, t), \quad (53)$$

$$-w^{29}t^4R_{1,2}^{-1} = T_{1,2}(w, t)Q_{1,2}(w, t), \quad (54)$$

where

$$T_{1,-2}(w, t) = T_{1,2}(w, t) = (w^2 + 1)(w^2 + w + 1)(1 - w)^2(w + 1)^2(1 + t)(1 - t)^2, \quad (55)$$

$$\begin{aligned} T_{1,-1}(w, t) &= T_{1,1}(w, t)s = (w + 1)(w^2 + w + 1)(1 - w)^2 \\ &\quad \times (1 + t)(t^2 + t + 1)(1 - t)^4, \end{aligned} \quad (56)$$

$$T_{1,0}(w, t) = (1 - w)^2(w + 1)^2(1 + t)(t^2 + t + 1)(1 - t)^2 \quad (57)$$

and

$$\begin{aligned} Q_{1,-2} &= (1 - tw)(1 - tw^2)(t - w)(t - w^3)(t - w^4)(t - w^5)(t - w^6) \\ &\quad \times (t^2 - w)(t^2 - w^2)(t^2 - w^3)(t^2 - w^4)(t^3 - w^2)(t^3 - w^3)(t^3 - w^4) \\ &\quad \times (t^3 - w^5)(t^3 - w^6) \end{aligned} \quad (58)$$

$$\begin{aligned} Q_{1,-1} &= (1 - tw)(1 - tw^2)(1 - t^2w)(t - w^2)^2(t - w^3)(t - w^4)(t^2 - w) \\ &\quad \times (t^2 - w^2)(t^2 - w^3)(t^3 - w)(t^3 - w^2)(t^3 - w^3)(t^3 - w^4) \end{aligned} \quad (59)$$

$$\begin{aligned} Q_{1,0} &= (1 - tw)^2(1 - tw^2)^2(1 - t^2w)(1 - t^2w^2)(1 - t^3w)(1 - t^3w^2)(t - w)^2 \\ &\quad \times (t - w^2)^2(t^2 - w)(t^2 - w^2)(t^3 - w)(t^3 - w^2) \end{aligned} \quad (60)$$

$$\begin{aligned} Q_{1,1} &= (1 - tw^2)^2(1 - tw^3)(1 - tw^4)(1 - t^2w)(1 - t^2w^2)(1 - t^2w^3) \\ &\quad \times (1 - t^3w)(1 - t^3w^2)(1 - t^3w^3)(1 - t^3w^4)(t - w)(t - w^2)(t^2 - w) \end{aligned} \quad (61)$$

$$\begin{aligned} Q_{1,2} &= (1 - tw)(1 - tw^3)(1 - tw^4)(1 - tw^5)(1 - tw^6)(1 - t^2w)(1 - t^2w^2) \\ &\quad \times (1 - t^2w^3)(1 - t^2w^4)(1 - t^3w^2)(1 - t^3w^3)(1 - t^3w^4)(1 - t^3w^5) \\ &\quad \times (1 - t^3w^6)(t - w)(t - w^2). \end{aligned} \quad (62)$$

$$\boxed{n = 2}$$

$$w^{17}P_{2,-2}(w, t)R_{2,-2}^{-1} = T_{2,-2}(w, t)Q_{2,-2}(w, t), \quad (63)$$

$$w^{14}P_{2,-1}(w, t)R_{2,-1}^{-1} = T_{2,-1}(w, t)Q_{2,-1}(w, t), \quad (64)$$

$$w^{13}P_{2,0}(w, t)R_{2,0}^{-1} = T_{2,0}(w, t)Q_{2,0}(w, t), \quad (65)$$

$$w^{14}P_{2,1}(w, t)R_{2,1}^{-1} = T_{2,1}(w, t)Q_{2,1}(w, t), \quad (66)$$

$$w^{17}P_{2,2}(w, t)R_{2,2}^{-1} = T_{2,2}(w, t)Q_{2,2}(w, t), \quad (67)$$

where

$$\begin{aligned} T_{2,-2}(w, t) = T_{2,2}(w, t) &= (w^2 + 1)(w^2 + w + 1)(w - 1)^2(w + 1)^2(1 + t) \\ &\times (t^2 + t + 1)(-1 + t)^4 \end{aligned} \quad (68)$$

$$T_{2,-1}(w, t) = T_{2,1}(w, t) = (w + 1)(w^2 + w + 1)(w - 1)^2(1 + t)(1 - t)^2 \quad (69)$$

$$T_{2,0}(w, t) = (1 - w)^2(w + 1)^2(1 + t)(t^2 + t + 1)(1 - t)^2 \quad (70)$$

and

$$\begin{aligned} Q_{2,-2} &= (1 - tw)(1 - tw^2)^2(1 - tw^4)(1 - tw^6)(1 - t^3w^2)(t - w)(t^2 - w) \\ &\times (t^2 - w^2)(t^2 - w^3)(t^2 - w^4)(t^3 - w^2)(t^3 - w^4)(t^3 - w^6) \end{aligned} \quad (71)$$

$$\begin{aligned} Q_{2,-1} &= (1 - tw)^2(1 - tw^2)(1 - tw^3)(1 - tw^5)(1 - t^2w)(1 - t^3w)(1 - t^3w^3) \\ &\times (t - w^2)(t - w^3)(t^2 - w)(t^2 - w^2)(t^2 - w^3) \\ &\times (t^3 - w)(t^3 - w^3)(t^3 - w^5) \end{aligned} \quad (72)$$

$$\begin{aligned} Q_{2,0} &= (1 - tw)(1 - tw^2)^2(1 - tw^4)(1 - t^2w)(1 - t^2w^2)(1 - t^3w^2)(1 - t^3w^4) \\ &\times (t - w)(t - w^2)^2(t - w^4)(t^2 - w)(t^2 - w^2)(t^3 - w^2)(t^3 - w^4) \end{aligned} \quad (73)$$

$$\begin{aligned} Q_{2,1} &= (1 - tw^2)(1 - tw^3)(1 - t^2w)(1 - t^2w^2)(1 - t^2w^3) \\ &\times (1 - t^3w)(1 - t^3w^3)(1 - t^3w^5)(t - w)^2(t - w^2)(t - w^3)(t - w^5) \\ &\times (t^2 - w)(t^3 - w)(t^3 - w^3) \end{aligned} \quad (74)$$

$$\begin{aligned} Q_{2,2} &= (1 - tw)(1 - t^2w)(1 - t^2w^2)(1 - t^2w^3)(1 - t^2w^4)(1 - t^3w^2)(1 - t^3w^4) \\ &\times (1 - t^3w^6)(t - w)(t - w^2)^2(t - w^4)(t - w^6)(t^3 - w^2), \end{aligned} \quad (75)$$

while the $P_{2,k}(w, t)$ are irreducible polynomials in w, t of total degree up to 18 which we do not display here.

For the purposes of this exposition, the important information lies in the $Q_{1,k}$ and $Q_{2,k}$ which indicate the points w inside the unit circle at which residues will need to be evaluated.

Table 2. Table of values (p, q) for which the factor $(t^q - w^p)$ occurs in $Q_{j,k}$ for $j=1,2$ and $k = -2 \dots 2$.

$Q_{1,-2}$	(1,1),	(3,1),	(4,1),	(5,1),	(6,1),	(1,2),	(2,2),	(3,2),	(4,2),	(2,3),	(3,3),	(4,3),	(5,3),	(6,3)
$Q_{1,-1}$	(2,1),	(3,1),	(4,1),			(1,2),	(2,2),	(3,2),		(1,3),	(2,3),	(3,3),	(4,3)	
$Q_{1,0}$	(1,1),	(2,1),				(1,2),	(2,2),			(1,3),	(2,3)			
$Q_{1,1}$	(1,1),	(2,1),				(1,2)								
$Q_{1,2}$	(1,1),	(2,1)												
$Q_{2,-2}$	(1,1),					(1,2),	(2,2),	(3,2),	(4,2),	(2,3),		(4,3),		(6,3)
$Q_{2,-1}$	(2,1),	(3,1),				(1,2),	(2,2),	(3,2),		(1,3),		(3,3),		(5,3)
$Q_{2,0}$	(1,1),	(2,1),	(4,1),			(1,2),	(2,2),			(2,3),		(4,3)		
$Q_{2,1}$	(1,1),	(2,1),	(3,1),	(5,1),		(1,2),				(1,3),		(3,3)		
$Q_{2,2}$	(1,1),	(2,1),	(4,1),	(6,1),						(2,3)				

The relevant factors are those of the form $(t^q - w^p)$ for positive integers p, q . We list in table 2 the values of (p, q) corresponding to each $Q_{j,k}$.

We next need to evaluate the residues of

$$F(w, t) = \sum_{k=-2}^2 R_{1,k}(w, t) + \sum_{k=-2}^2 R_{2,k}(w, t) \quad (76)$$

at the singularities w lying inside the unit circle $|w| = 1$, where $|t| < 1$. It is helpful to note that some of the relevant factors in the denominators of the $R_{j,k}$ no longer appear when the $R_{j,k}$ are summed and simplified. In fact it turns out that

$$F(w, t) = 2w^{13}(1 - w)^2 \frac{P(w, t)}{Q(w, t)}, \quad (77)$$

where $P(w, t)$ is an irreducible polynomial in w, t of total degree 55 and integer coefficients, while

$$\begin{aligned} Q(w, t) = (\dots)(t - w)(t^2 - w)(t^2 - w^2)(t^2 - w^3)(t^2 - w^4)(t^3 - w)(t^3 - w^2) \\ \times (t^3 - w^3)(t^3 - w^4)(t^3 - w^5)(t^3 - w^6) \end{aligned} \quad (78)$$

with the dots (\dots) representing factors involving t only or otherwise not vanishing for w inside the unit circle. Note that factors with $(p, q) = (m, 1)$ for $3 \leq m \leq 6$ do not arise here although they do appear in table 1: the residues of the individual $R_{j,k}$ corresponding to these factors sum to zero. The case $(p, q) = (2, 1)$ also does not appear explicitly in $Q(w, t)$, although $(t - w^2)$ is a factor of both $(t^2 - w^4)$ and $(t^3 - w^6)$ and so the ‘virtual’ case $(2, 1)$ needs to be considered.

2.6.2. Residues of the w -singularities. We now evaluate the residues of $F(w, t)$ at the singularities w that lie inside the unit circle, dealing with each case (p, q) in turn. We write $W_{p,q}(t)$ for the sum of the residues at those points w where $w^p = t^q$, excluding those already found from any earlier (p', q') with $p/q = p'/q'$

$$\boxed{(p, q) = (1, 1)}$$

$$W_{1,1}(t) = \frac{t^4 U_{1,1}(t)}{36 V_{1,1}(t)}, \quad (79)$$

where $U_{1,1}(t)$ is a palindromic polynomial in t of degree 56 with positive integer coefficients, and

$$\begin{aligned} V_{1,1}(t) = (1 - t)(1 - t^2)^3(1 - t^3)^2(1 - t^4)^3(1 - t^5)^3(1 - t^6)^3 \\ \times (1 - t^7)^2(1 - t^8)(1 - t^9). \end{aligned} \quad (80)$$

$$\boxed{(p, q) = (2, 1)}$$

$$W_{2,1}(t) = \frac{U_{2,1}(t)}{6 V_{2,1}(t)}, \quad (81)$$

where $U_{2,1}(t)$ is a palindromic polynomial in t of degree 60 with positive integer coefficients, and

$$V_{2,1}(t) = (1-t)^2(1-t^2)^2(1-t^3)^4(1-t^4)^3(1-t^5)^3(1-t^6) \\ \times (1-t^7)^2(1-t^9)(1-t^{11}). \quad (82)$$

$$\boxed{(p, q) = (1, 2)}$$

$$W_{1,2}(t) = -\frac{2t^{19}U_{1,2}(t)}{V_{1,2}(t)}, \quad (83)$$

where $U_{1,2}(t)$ is a palindromic polynomial in t of degree 46 with positive integer coefficients, and

$$V_{1,2}(t) = (1-t)^2(1-t^2)(1-t^3)^2(1-t^4)^2(1-t^5)^3(1-t^6)^2(1-t^7)^2 \\ \times (1-t^8)(1-t^9)^2(1-t^{11})(1-t^{13}). \quad (84)$$

$\boxed{(p, q) = (2, 2)}$ excluding residues already occurring at $(p, q) = (1, 1)$:

$$W_{2,2}(t) = -\frac{t^4 U_{2,2}(t)}{4 V_{2,2}(t)}, \quad (85)$$

where $U_{2,2}(t)$ is a palindromic polynomial in t of degree 20 with positive integer coefficients, and

$$V_{2,2}(t) = (1-t)^2(1-t^2)(1-t^3)(1-t^4)^2(1-t^5)(1-t^6)(1-t^7) \\ \times (1-t^8)(1-t^{12}). \quad (86)$$

$\boxed{(p, q) = (3, 2)}$ Here the calculations are simplified by noting that $(3, 2)$ appears in table 1 only where $k = -2, -1$. It also turns out that the $(3, 2)$ residue sum for $R_{j,-2}$ is equal to that for $R_{j,-1}$, $j = 1, 2$. We find

$$W_{3,2} = \frac{2t^2 U_{3,2}}{V_{3,2}}, \quad (87)$$

where $U_{3,2}(t)$ is a palindromic polynomial in t of degree 54 with positive integer coefficients, and

$$V_{3,2}(t) = (1-t)^5(1-t^2)^3(1-t^3)(1-t^4)^2(1-t^5)^3(1-t^7)^2(1-t^8) \\ \times (1-t^{11})(1-t^{13}). \quad (88)$$

$\boxed{(p, q) = (4, 2)}$ Here $(4, 2)$ appears in table 1 only where $k = -2$. Excluding residues already occurring at $(p, q) = (2, 1)$ we find

$$W_{4,2} = \frac{U_{4,2}}{2 V_{4,2}}, \quad (89)$$

where $U_{4,2}(t)$ is a palindromic polynomial in t of degree 8 with positive integer coefficients, and

$$V_{4,2}(t) = (1+t)^3(1-t^2)(1+t^3)^2(1-t^4)^2(1-t^6)(1-t^8). \quad (90)$$

$$\boxed{(p, q) = (1, 3)}$$

$$W_{1,3} = \frac{2t^{32}U_{1,3}}{V_{1,3}}, \quad (91)$$

where $U_{1,3}(t)$ is a palindromic polynomial in t of degree 16 with positive integer coefficients, and

$$V_{1,3}(t) = (1 - t^2)^3(1 - t^3)(1 - t^4)^3(1 - t^5)^3(1 - t^6)^3(1 - t^7)^2(1 - t^8) \\ \times (1 - t^9)^2(1 - t^{11}). \quad (92)$$

$$\boxed{(p, q) = (2, 3)}$$

$$W_{2,3} = \frac{2t^{11}U_{2,3}}{V_{2,3}}, \quad (93)$$

where $U_{2,3}(t)$ is a palindromic polynomial in t of degree 52 with positive integer coefficients, and

$$V_{2,3}(t) = (1 - t)^3(1 - t^2)(1 - t^3)^2(1 - t^4)^2(1 - t^5)^3(1 - t^6)^2(1 - t^7)^2 \\ \times (1 - t^8)(1 - t^9)^2(1 - t^{13}). \quad (94)$$

$$\boxed{(p, q) = (3, 3)} \text{ excluding residues already occurring at } (p, q) = (1, 1):$$

$$W_{3,3} = \frac{2t^4(1 + t)(1 + t^2)U_{3,3}}{9V_{3,3}}, \quad (95)$$

where $U_{3,3}(t)$ is a palindromic polynomial in t of degree 14 with positive integer coefficients, and

$$V_{3,3}(t) = (1 - t^3)(1 - t^5)(1 - t^6)^2(1 - t^9)^2(1 - t^{12}). \quad (96)$$

$$\boxed{(p, q) = (4, 3)}$$

$$W_{4,3} = -\frac{2t^2U_{4,3}}{V_{4,3}}, \quad (97)$$

where $U_{4,3}(t)$ is a palindromic polynomial in t of degree 50 with positive integer coefficients, and

$$V_{4,3}(t) = (1 - t)^5(1 - t^2)^2(1 - t^3)^4(1 - t^5)^3(1 - t^7)^2(1 - t^9)^2(1 - t^{11}). \quad (98)$$

$$\boxed{(p, q) = (5, 3)}$$

$$W_{5,3} = -\frac{2t U_{5,3}}{V_{5,3}}, \quad (99)$$

where $U_{5,3}(t)$ is a palindromic polynomial in t of degree 82 with positive integer coefficients, and

$$V_{5,3}(t) = (1-t)^2(1-t^2)^4(1-t^3)(1-t^4)^2(1-t^6)^2(1-t^7)^2(1-t^8)(1-t^9)^2 \\ \times (1-t^{11})(1-t^{12})(1-t^{13}). \quad (100)$$

$\overline{(p, q)} = (6, 3)$ The factor $(w^6 - t^3)$ appears in $R_{j,k}$ only for $k = -2$, and the residue sums (excluding those already obtained at $(p, q) = (2, 1)$) for $R_{1,-2}$ and for $R_{2,-2}$ coincide and give

$$W_{6,3} = \frac{4 U_{6,3}}{3 V_{6,3}}, \quad (101)$$

where $U_{6,3}(t)$ is a palindromic polynomial in t of degree 12 with positive integer coefficients, and

$$V_{6,3}(t) = (1-t)(1-t^3)^2(1-t^6)^2(1-t^9)^2. \quad (102)$$

Finally, adding all these residues yields the following result.

Proposition 3. *The sum $W(t)$ of all the residues of $F(w, t)$ for $|w| < 1$ (where $|t| < 1$) has the form*

$$W(t) = 4 \frac{U(t)}{V(t)}, \quad (103)$$

where $U(t)$ is a palindromic polynomial in t of degree 96 with integer coefficients and

$$V(t) = (1+t)(1-t^2)^3(1-t^3)(1-t^4)^2(1-t^5)^3(1-t^6)^2(1-t^7)^2(1-t^8) \\ \times (1-t^9)^2(1-t^{11})(1-t^{12})(1-t^{13}). \quad (104)$$

The algebraic form of $W(t)$ is somewhat anomalous for this context, as the coefficients in the numerator $U(t)$ are not all positive, and the denominator $V(t)$ has an apparently superfluous factor $(1+t)$. Nevertheless, the total number of other factors (with repeats) is 19 which is the codimension 25–6 of the generic orbits of the group action as would be expected. In fact expansion as a power series in t yields a pleasing result.

Theorem 1. *The Molien series $\mathcal{P}_{\Gamma_0}^2(t)$ for the action of $\Gamma_0 = \mathbf{SO}(3) \times \mathbf{SO}(3)$ on $L(V^*, V) \cong \mathbf{R}^{25}$ is given by*

$$\mathcal{P}_{\Gamma_0}^2(t) = 1 + t^2 + t^3 + 5t^4 + 5t^5 + 19t^6 + 27t^7 + 76t^8 + 136t^9 + 330t^{10} + 626t^{11} \\ + 1391t^{12} + 2676t^{13} + 5497t^{14} + 10425t^{15} + 20201t^{16} + 37182t^{17} \\ + 68713t^{18} + 122489t^{19} + 217275t^{20} + O(t^{21}). \quad (105)$$

This form with positive integer coefficients suggests that suitable algebraic manipulation of $W(t)$ ought to put this rational function into a form consistent with data for primary and secondary generators of the ring of Γ_0 -invariants. We are grateful to Boris Zhilinskii who showed us how to arrive at the following more informative conclusion.

Theorem 2. An admissible expression of the Molien function $\mathcal{P}_{I_0}^2(t)$ for the action of $I_0 = \mathbf{SO}(3) \times \mathbf{SO}(3)$ on $L(V^*, V) \cong \mathbf{R}^{25}$ is given by

$$\mathcal{P}_{I_0}^2(t) = \frac{R_0(t)}{Q_0(t)}, \quad (106)$$

where

$$\begin{aligned} Q_0(t) = & (1 - t^2)(1 - t^3)(1 - t^4)^3(1 - t^5)(1 - t^6)^2(1 - t^7)^2(1 - t^8)^2 \\ & \times (1 - t^9)^2(1 - t^{10})^2(1 - t^{11})(1 - t^{12})(1 - t^{13}) \end{aligned} \quad (107)$$

and $R_0(t)$ is a palindromic polynomial in t of degree 113 with positive integer coefficients as set out in appendix A.

As discussed above at the start of section 2, an admissible rational expression of a given Molien series is far from unique. However, the Molien power series defines a meromorphic function on \mathbf{C} with zeros and poles of well-defined orders. Expressing such a function in a completely reduced form $P^*(t)/Q^*(t)$ where P^* , Q^* (unique up to sign) have integer coefficients and no common factors we see that any admissible rational expression $P(t)/Q(t)$ for the given Molien series has $P/P^* = Q/Q^* = J(t)$ for some polynomial J ; moreover, $J(1) \neq 0$ since $P(1) > 0$. In particular, if $P(t)/Q(t)$ is the ‘correct’ rational expression in which $Q(t)$ as in (18) indicates the degrees d_i of the primary generators of \mathcal{R} while the coefficients of $P(t)$ give the numbers of secondary generators at each degree, then we see that the total number of secondary generators is $J(1)P^*(1)$. In our case we find $R_0(t) = J_0(t)P^*(t)$ with

$$J_0(t) = (1 + t)(1 + t^2)^2(1 + t^4)(1 - t + t^2 - t^3 + t^4)^2$$

and $P^*(1) = 181\,740\,756$. We conclude that the number of secondary invariants is an integer multiple of this number, while Q^* has a zero of order 19 at $t = 1$ and therefore there are 19 primary invariants.

We now turn to the Molien integral (30) for the full group $\Gamma = \mathbf{SO}(3) \wr \mathbf{Z}_2$ in the $\ell = 2$ case. It follows from (35) and (36) that we must evaluate the residues at singularities inside the unit circle of the function

$$H(w, t) := \frac{(1 - v)^2}{v^2 K(v, t)} \quad (108)$$

with $K(v, t)$ as in (36), namely at the points $v = t^2, \pm t, \pm \sqrt{t}$ and $\exp(2\pi i/3)t^{\frac{2}{3}}$ for $m = 0, 1, 2$, and finally divide by the factor $(1 - t)^3(1 + t)^2$. We arrive at the following result.

Proposition 4.

$$\mathcal{P}_{I_1}^2(t) = \frac{U_1(t)}{V_1(t)},$$

where $U_1(t)$ is a palindromic polynomial in t of degree 42 with integer coefficients

$$\begin{aligned} U_1(t) = & 1 - t + 2t^2 - 3t^3 + 3t^4 - t^5 + 4t^6 + 4t^7 + 6t^8 + 13t^9 + 10t^{10} \\ & + 24t^{11} + 19t^{12} + 35t^{13} + 34t^{14} + 45t^{15} + 53t^{16} + 58t^{17} + 69t^{18} + 65t^{19} + 81t^{20} \\ & + 69t^{21} + 81t^{22} + 65t^{23} + 69t^{24} + 58t^{25} + 53t^{26} + 45t^{27} + 34t^{28} + 35t^{29} + 19t^{30} \\ & + 24t^{31} + 10t^{32} + 13t^{33} + 6t^{34} + 4t^{35} + 4t^{36} - t^{37} + 3t^{38} - 3t^{39} \\ & + 2t^{40} - t^{41} + t^{42}, \end{aligned} \quad (109)$$

and

$$\begin{aligned} V_1(t) = & (1 + t^2)(1 - t)(1 - t^3)^2(1 - t^4)^2(1 - t^5)(1 - t^6)^2(1 - t^7) \\ & \times (1 - t^8)^2(1 - t^{10}). \end{aligned} \quad (110)$$

Again this may be put into a more propitious form

$$\mathcal{P}_{\Gamma_1}^2(t) = \frac{R_1(t)}{Q_1(t)}, \quad (111)$$

where $Q_1(t) = Q_0(t)$ and where $R_1(t)$ is a polynomial in t of degree 113 which is palindromic up to sign-reflection as also given in appendix A. Here $P_1(t) = U_1(t)$. $Q_0(t)/V_1(t)$ and

$$\begin{aligned} Q_0(t)/V_1(t) = & (1 + t)(1 - t^2)(1 + t^3 + t^6)(1 - t^7)(1 - t^9) \\ & \times (1 - t^{10})(1 - t^{11})(1 - t^{12})(1 - t^{13}). \end{aligned} \quad (112)$$

Expanding $\mathcal{P}_{\Gamma_1}^2(t)$ as a power series in t we find

$$\begin{aligned} \mathcal{P}_{\Gamma_1}^2(t) = & 1 + t^2 + t^3 + 3t^4 + 5t^5 + 9t^6 + 13t^7 + 28t^8 + 44t^9 + 72t^{10} + 116t^{11} \\ & + 193t^{12} + 294t^{13} + 457t^{14} + 689t^{15} + 1039t^{16} + 1526t^{17} \\ & + 2221t^{18} + 3177t^{19} + 4541t^{20} + O(t^{21}) \end{aligned} \quad (113)$$

which finally gives the Molien series for Γ as the arithmetic mean of (105) and (113) as follows:

Theorem 3.

$$\begin{aligned} \mathcal{P}_{\Gamma}^2(t) = & 1 + t^2 + t^3 + 4t^4 + 5t^5 + 14t^6 + 20t^7 + 52t^8 + 90t^9 + 201t^{10} + 371t^{11} \\ & + 792t^{12} + 1485t^{13} + 2977t^{14} + 5557t^{15} + 10\,620t^{16} + 19\,354t^{17} \\ & + 35\,467t^{18} + 62\,833t^{19} + 110\,908t^{20} + O(t^{21}). \end{aligned} \quad (114)$$

Observe that (as must be the case since $\Gamma_0 < \Gamma$) the positive integer coefficients in \mathcal{P}_{Γ}^2 are less than or equal to the corresponding coefficients in $\mathcal{P}_{\Gamma_0}^2(t)$ as in theorem 1: their difference at degree n is the number of independent homogeneous invariants of degree n for Γ_0 which change their sign under the transposition action. We examine this a little more closely in the following section.

The series (114) can be given an admissible rational expression with denominator $Q_0(t)$ and numerator $P_2(t) = \frac{1}{2}(R_0(t) + R_1(t))$. Here we find $P_2(t) = J_2(t)\tilde{P}^*(t)$ with \tilde{P}^* irreducible

over the integers and

$$J_2(t) = (1+t)(1+t^2)(1-t+t^2-t^3+t^4).$$

We conclude that the total number of secondary invariants for the whole group Γ is therefore an integer multiple of $\tilde{P}^*(1) = 363, 481, 512$. If we knew $P_2(t)/Q_0(t)$ to be the ‘correct’ expression in terms of generators for the ring of polynomial invariants then since $J_2(1) = 4$ we could conclude that the number of secondary invariants is $P_2(1) = 4\tilde{P}^*(1) = 1\,453\,926\,048$.

3. The algebra of irreducible super-tensors

3.1. Tensor products and invariants

The tensor product of two (complex) unitary representations D, D' of a compact Lie group \mathbf{G} on linear spaces V, V' of dimension n, n' respectively is (as is any other) isomorphic to a direct sum of irreducible representations of \mathbf{G} :

$$D \otimes D' \cong D_0 \oplus D_1 \cdots \oplus D_m. \quad (115)$$

Explicitly this means that with respect to a chosen basis of $V \otimes V'$ there is a unitary $nn' \times nn'$ matrix C , independent of $g \in \mathbf{G}$, such that

$$C(D(g) \otimes D'(g))C^* = \text{diag}(D_0(g), D_1(g), \dots, D_m(g)) \quad (116)$$

for all $g \in \mathbf{G}$, where the right hand side is a block-diagonal matrix.

Suppose that D_0 is the trivial one-dimensional representation of \mathbf{G} , and that it appears precisely once in (116). Orthogonal projection of $V \otimes V'$ onto its one-dimensional \mathbf{G} -invariant linear subspace corresponding to D_0 is a \mathbf{G} -invariant linear function on $V \otimes V'$, which in the case $V = V'$ gives a quadratic \mathbf{G} -invariant function on V . More generally, for $k = 0, \dots, m$ the orthogonal projection of $V \otimes V'$ onto its invariant n_k -dimensional subspace V_k supporting the representation D_k is an equivariant linear map given by the $n_k \times nn'$ matrix C_k consisting of the n_k rows of C corresponding to the D_k -block. Using this projection and iterating the procedure with higher order tensor products using (116) provides a systematic method for finding higher order invariants. We illustrate the use of this method below.

For our purposes we need to extend these considerations to the situation where V, V' are replaced by $L(W^*, V), L(W'^*, V')$ for further representation spaces W, W' for \mathbf{G} . In view of the natural identification

$$L(W^* \otimes W'^*, V \otimes V') \cong L(W^*, V) \otimes L(W'^*, V') \quad (117)$$

for linear spaces V, W, V', W' through which the element $A \otimes B$ on the right hand side corresponds to the linear map

$$W^* \otimes W'^* \rightarrow V \otimes V': w^* \otimes w'^* \mapsto Aw^* \otimes Bw'^* \quad (118)$$

on the left hand side, the tensor product representation $D \otimes D'$ of \mathbf{G} on $V \otimes V'$ defines a natural action of \mathbf{G} on $L(W^*, V) \otimes L(W'^*, V')$ by left multiplication (right composition) on $L(W^* \otimes W'^*, V \otimes V')$, and similarly two representations E, E' of \mathbf{G} on W, W' define a \mathbf{G} -action on $L(W^*, V) \otimes L(W'^*, V')$ by right dual multiplication (left dual composition). Schematically, we have for $S \in L(W^*, V)$ and $S' \in L(W'^*, V')$:

$$\begin{array}{ccc}
W^* & \xrightarrow{S} & V \\
\uparrow E(h)^* & & \downarrow D(g) \\
W^* & \xrightarrow{(g,h)S} & V
\end{array}
\quad
\begin{array}{ccc}
W'^* & \xrightarrow{S'} & V' \\
\uparrow E'(h)^* & & \downarrow D'(g) \\
W'^* & \xrightarrow{(g,h)S'} & V'
\end{array}$$

Together these define a representation of $\mathbf{G} \times \mathbf{G}$ on $L(W^*, V) \otimes L(W'^*, V')$ given explicitly by

$$\begin{aligned}
(g, h): S \otimes S' &\mapsto [D(g)SE^*(h)] \otimes [D'(g)S'E'^*(h)] \\
&= [D(g) \otimes D'(g)](S \otimes S')[E^*(h) \otimes E'^*(h)]. \quad (119)
\end{aligned}$$

Stated otherwise, the following diagram commutes:

$$\begin{array}{ccc}
W^* \otimes W'^* & \xrightarrow{S \otimes S'} & V \otimes V' \\
\uparrow E(h)^* \otimes E'(h)^* & & \downarrow D(g) \otimes D'(g) \\
W^* \otimes W'^* & \xrightarrow{(g,h)(S \otimes S')} & V \otimes V'
\end{array}$$

Let the projections $\{B_\ell: W \otimes W' \rightarrow W_\ell\}$ be analogs for $E \otimes E'$ of the projections $\{C_k: V \otimes V' \rightarrow V_k\}$ for $D \otimes D'$ described above.

Lemma 1. *For each pair k, ℓ the linear map*

$$\Phi_{k\ell}: L(W^*, V) \otimes L(W'^*, V') \rightarrow L(W_\ell^*, V_k): S \otimes S' \mapsto C_k S \otimes S' B_\ell^*$$

is $\mathbf{G} \times \mathbf{G}$ -equivariant.

Proof. From the expression (116) we have

$$C_k(D(g) \otimes D'(g)) = D_k(g)C_k$$

and likewise

$$(E^*(g) \otimes E'^*(g))B_\ell^* = B_\ell^* E_\ell^*(g)$$

for each pair k, ℓ . Therefore for $(g, h) \in \mathbf{G} \times \mathbf{G}$ we have

$$\begin{aligned}
\Phi_{k\ell}((g, h)S \otimes S') &= C_k[D(g) \otimes D'(g)](S \otimes S')[E^*(h) \otimes E'^*(h)]B_\ell^* \\
&= D_k(g)C_k(S \otimes S')B_\ell^* E_\ell^*(h) \\
&= (g, h)\Phi_{k\ell}(S \otimes S').
\end{aligned}$$

We shall apply this in the case of $\mathbf{G} = \mathbf{SO}(3)$ with $V = V' = W = W' \cong \mathbf{R}^5$ and with D, D', E, E' all given by the $j = 2$ irreducible representation $D^{(2)}$. The $j = 0$ component of (119) defined by Φ_{00} yields a quadratic invariant for the action of $\mathbf{SO}(3) \times \mathbf{SO}(3)$ on

$L(V^*, V)$, and we show how further iteration of this construction yields explicit invariants of degree 3 and 4.

3.2. The case of $\mathbf{SO}(3)$ and Clebsch–Gordan coefficients

The context in which $\mathbf{G} = \mathbf{SO}(3)$ and D, D' are irreducible is thoroughly studied in the quantum mechanics literature [2, 19, 20]. If $D = D^{(j_1)}$ and $D' = D^{(j_2)}$ where $D^{(j_1)}, D^{(j_2)}$ are the unique irreducible representations on linear spaces $V^{(j_1)}, V^{(j_2)}$ of dimension $2j_1 + 1, 2j_2 + 1$ respectively, then the *Clebsch–Gordan formula or series* [1, 21] states that

$$D^{(j_1)} \otimes D^{(j_2)} \cong D^{(|j_1 - j_2|)} \oplus D^{(|j_1 - j_2| + 1)} \oplus \dots \oplus D^{(j_1 + j_2)} \quad (120)$$

or, more explicitly, that with spherical harmonics Y_{jm} , $m = -j, \dots, j$ chosen as a basis for $V^{(j)}$ and giving the basis $\{Y_{j_1 m_1} \otimes Y_{j_2 m_2}\}$ for $V^{(j_1)} \otimes V^{(j_2)}$ there exists a unique unitary $N \times N$ matrix C , where $N = (2j_1 + 1)(2j_2 + 1)$, such that

$$C \left[D^{(j_1)} \otimes D^{(j_2)} \right] C^* = \begin{pmatrix} D^{(|j_1 - j_2|)} & 0 & \dots & 0 \\ 0 & D^{(|j_1 - j_2| + 1)} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & D^{(j_1 + j_2)} \end{pmatrix} \quad (121)$$

where the matrix $D^{(j)}$ is called the Wigner rotation matrix of rank j [2]. The entries of the matrix C are known as *Clebsch–Gordan coefficients* [20, 21] and are usually written as

$$C_{jm; m_1 m_2} = \langle jm | j_1 m_1; j_2 m_2 \rangle, \quad (122)$$

where for fixed j_1, j_2 the pairs of indices j, m and m_1, m_2 label rows and columns respectively. These coefficients vanish unless

$$|j_1 - j_2| \leq j \leq j_1 + j_2, \quad m_1 + m_2 = m \quad (123a)$$

$$-j_1 \leq m_1 \leq j_1, \quad -j_2 \leq m_2 \leq j_2, \quad -j \leq m \leq j. \quad (123b)$$

Note that the right hand side of (120) includes the trivial one-dimensional representation $D^{(0)}$ if and only if $j_1 = j_2$.

The use of the explicit matrix representation in terms of spherical harmonics is particularly convenient since many detailed results are readily available in the quantum mechanics literature. For later reference it is also useful to introduce the more symmetric Wigner 3- j symbols [19, 20] defined as

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m_3}}{\sqrt{2j_3 + 1}} \langle j_3 (-m_3) | j_1 m_1; j_2 m_2 \rangle. \quad (124)$$

These vanish unless

$$m_1 + m_2 + m_3 = 0, \quad |j_1 - j_2| \leq j_3 \leq j_1 + j_2. \quad (125)$$

Finally, we record the following special case of the Clebsch–Gordan coefficients

$$\begin{pmatrix} j_1 & j_2 & 0 \\ m_1 & m_2 & 0 \end{pmatrix} = \langle 00 | j_1 m_1; j_2 m_2 \rangle = \delta_{j_1 j_2} \delta_{m_1, -m_2} \frac{(-1)^{j_1 - m_1}}{\sqrt{2j_1 + 1}}, \quad (126)$$

where $\delta_{h,k}$ is the Kronecker symbol equal to 1 if $h = k$ and zero otherwise. We refer to any standard textbook on quantum mechanics for a more complete review of the numerous interesting identities and symmetries of Clebsch–Gordan coefficients and 3-j symbols.

3.3. Construction of invariants for the $\mathbf{SO}(3) \times \mathbf{SO}(3)$ -action on $L(V^{(2)}, V^{(2)})$

We now focus on the case $j_1 = j_2 = 2$. Let C_j denote the rectangular matrix obtained from C by selecting the $(2j + 1)$ -rows associated with the j th block in (121), so that C_j has dimensions $(2j + 1) \times 25$. Taking $j = 0$ (so $m = 0$) and using (123a) we see from lemma 1 with $k, \ell = 0, 0$ and equation (126) that for $S \in L(V^{(2)}, V^{(2)})$

$$\begin{aligned}\Phi_{00}(S \otimes S) &= \sum_{m,m'} (-1)^{m+m'} \langle 00 | 2m_1; 2m_2 \rangle \langle 00 | 2m'_1; 2m'_2 \rangle S_{m_1 m'_1} S_{m_2 m'_2} \\ &= \frac{1}{5} \sum_{m,m'} (-1)^{m+m'} S_{mm'} S_{-m -m'},\end{aligned}\quad (127)$$

with $-2 \leq m, m' \leq 2$. Furthermore, since any Wigner rotation matrix $A = D^{(\ell)}$ automatically satisfies

$$A_{mm'}^* = (-1)^{m+m'} A_{-m -m'}$$

for $-\ell \leq m, m' \leq \ell$, the order parameter matrix S (obtained as an ensemble average over such A : see [7]) has the same properties and thus we immediately obtain

$$\Phi_{00}(S \otimes S) = I_2 := \|S\|^2, \quad (128)$$

as the expected quadratic invariant.

With a little more effort we can construct a cubic invariant. To this end, we apply the same process as above at degree 3 to obtain:

$$\begin{aligned}\Phi_{00}[\Phi_{jj'}(S \otimes S) \otimes S] &= \sum_{m,m',m_3,m'_3} \langle 00 | jm; 2m_3 \rangle \langle 00 | j'm'; 2m'_3 \rangle \\ &\quad \times [\Phi_{jj'}(S \otimes S)]_{mm'} S_{m_3 m'_3}.\end{aligned}\quad (129)$$

After the substitution of equation (126), we can see that the only non vanishing cubic invariant comes from the choice $j = j' = 2$. Thus, we obtain the following cubic invariant (see also [22]):

$$I_3 = \sum_{m_i, m'_i = -2}^2 \begin{pmatrix} 2 & 2 & 2 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} 2 & 2 & 2 \\ m'_1 & m'_2 & m'_3 \end{pmatrix} S_{m_1 m'_1} S_{m_2 m'_2} S_{m_3 m'_3}. \quad (130)$$

From the Molien series $\mathcal{P}_{I_0}^2$ in theorem 1 we expect a single generator for I_0 -invariants at each homogeneous degree 2 and 3, and so I_3 is the unique degree-3 invariant up to scalar multiplication. Moreover, we observe that I_2 and I_3 are clearly also invariant with respect to the transposition τ which exchanges m_i and m'_i . Therefore we conclude the following result.

Proposition 5. *The invariants I_2, I_3 generate the quadratic and the cubic invariants of the whole group $\Gamma \cong \mathbf{SO}(3) \wr \mathbf{Z}_2$.*

The structure of the invariants is, however, more involved at degree 4. To describe it more closely, let us first define the following super-tensors ($j, j' = 0, \dots, 4$)

$$U_{kk'}^{(j,j')} = \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ m_1 & m_2 & k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ m'_1 & m'_2 & k' \end{pmatrix} S_{m_1 m'_1} S_{m_2 m'_2}. \quad (131)$$

The $\mathbf{SO}(3) \times \mathbf{SO}(3)$ invariants of degree 4 can then be written as contractions (scalar product) of the $U^{(j,j')}$:

$$I_4^{(j,j')} = \sum_{\substack{|k| \leq j \\ |k'| \leq j'}} (-1)^{k+k'} U_{kk'}^{(j,j')} U_{-k,-k'}^{(j,j')}, \quad (132)$$

of which there are 25 since both j and j' range from 0 to 4. However, as we next show, these are not independent. Let us introduce the following definitions for the symmetric and skew-symmetric part of $I_4^{(j,j')}$:

$$I_4^{[j,j']} = \frac{1}{2} (I_4^{(j,j')} + I_4^{(j',j)}), \quad I_4^{\{j,j'\}} = \frac{1}{2} (I_4^{(j,j')} - I_4^{(j',j)}). \quad (133)$$

As described in detail in appendix B, the following general relations hold:

$$I_4^{(j,j')} = 0 \quad \text{if } j + j' \text{ is odd}, \quad (134a)$$

$$(I_4^{(j,j')})^* = I_4^{(j,j')}, \quad (134b)$$

$$\tau I_4^{[j,j']} = I_4^{[j,j']}, \quad \tau I_4^{\{j,j'\}} = -I_4^{\{j,j'\}}. \quad (134c)$$

There are 12 relations given by (134b) which reduces the number of potentially independent invariants (132) from 25 to 13. Moreover, as can be checked directly, the following less natural identities also hold:

$$4 I_4^{(0,0)} + 9 I_4^{(1,1)} + 5 I_4^{(2,2)} - 14 I_4^{(3,3)} - 54 I_4^{(4,4)} = 0, \quad (135a)$$

$$60 I_4^{(0,0)} + 9 I_4^{(1,1)} + 245 I_4^{(2,2)} - 784 I_4^{(3,3)} - 280 I_4^{[0,2]} = 0, \quad (135b)$$

$$212 I_4^{(0,0)} - 909 I_4^{(1,1)} + 2695 I_4^{(2,2)} - 3136 I_4^{(3,3)} - 1512 I_4^{[0,4]} = 0, \quad (135c)$$

$$100 I_4^{(0,0)} + 99 I_4^{(1,1)} - 1225 I_4^{(2,2)} + 784 I_4^{(3,3)} - 1008 I_4^{[1,3]} = 0, \quad (135d)$$

$$220 I_4^{(0,0)} - 387 I_4^{(1,1)} - 535 I_4^{(2,2)} + 112 I_4^{(3,3)} - 2160 I_4^{[2,4]} = 0, \quad (135e)$$

$$5 I_4^{[0,2]} - 9 I_4^{\{0,4\}} = 0, \quad (135f)$$

$$5 I_4^{\{0,2\}} - 6 I_4^{[1,3]} = 0, \quad (135g)$$

$$7 I_4^{[0,2]} + 18 I_4^{\{2,4\}} = 0. \quad (135h)$$

See appendix B for further details. These eight identities reduce the number of potentially independent degree-4 invariants from 13 to 5. From the Molien series $\mathcal{P}_{\Gamma_0}^2(t)$ in theorem 1 we expect to have five linearly independent degree-4 invariants of $\Gamma_0 = \mathbf{SO}(3) \times \mathbf{SO}(3)$, and we may accordingly take these to be $I_4^{(0,0)}$, $I_4^{(1,1)}$, $I_4^{(2,2)}$, $I_4^{(3,3)}$, $I_4^{[0,2]}$, say.

The relations (134c) show that, of these five invariants of Γ_0 , all except the last (which changes sign) are invariant under the transposition operator τ . This is consistent with the Molien series $\mathcal{P}_{\Gamma}^2(t)$ in theorem 3 which predicts only four linearly independent degree-4 invariants of $\mathbf{F} \mathbf{SO}(3) \wr \mathbf{Z}_2$. To summarize, we have established the following result:

Proposition 6. *The invariants $I_4^{(0,0)}$, $I_4^{(1,1)}$, $I_4^{(2,2)}$, $I_4^{(3,3)}$ generate the quartic invariants of the whole group $\Gamma \cong \mathbf{SO}(3) \wr \mathbf{Z}_2$.*

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Appendix A. Molien function details

The numerator $P_0(t)$ of the rational Molien function in theorem 2 is:

$$\begin{aligned}
 P_0(t) = & 1 + t^4 + 3t^5 + 11t^6 + 16t^7 + 42t^8 + 80t^9 + 185t^{10} + 357t^{11} + 752t^{12} \\
 & + 1412t^{13} + 2723t^{14} + 4937t^{15} + 8888t^{16} + 15342t^{17} + 26146t^{18} + 43083t^{19} \\
 & + 69884t^{20} + 110398t^{21} + 171406t^{22} + 260288t^{23} + 388723t^{24} + 569210t^{25} \\
 & + 820356t^{26} + 1161726t^{27} + 1620330t^{28} + 2224150t^{29} + 3009500t^{30} \\
 & + 4012238t^{31} + 5276926t^{32} + 6845013t^{33} + 8764870t^{34} + 11078260t^{35} \\
 & + 13830477t^{36} + 17054459t^{37} + 20782913t^{38} + 25029615t^{39} \\
 & + 29802829t^{40} + 35086893t^{41} + 40855850t^{42} + 47055721t^{43} + 53620919t^{44} \\
 & + 60456820t^{45} + 67458001t^{46} + 74494882t^{47} + 81431353t^{48} + 88115150t^{49} \\
 & + 94396925t^{50} + 100121953t^{51} + 105148447t^{52} + 109343460t^{53} + 112595858t^{54} \\
 & + 114815204t^{55} + 115941062t^{56} + 115941062t^{57} + 114815204t^{58} + 112595858t^{59} \\
 & + 109343460t^{60} + 105148447t^{61} + 100121953t^{62} + 94396925t^{63} + 88115150t^{64} \\
 & + 81431353t^{65} + 74494882t^{66} + 67458001t^{67} + 60456820t^{68} + 53620919t^{69} \\
 & + 47055721t^{70} + 40855850t^{71} + 35086893t^{72} + 29802829t^{73} + 25029615t^{74} \\
 & + 20782913t^{75} + 17054459t^{76} + 13830477t^{77} + 11078260t^{78} + 8764870t^{79} \\
 & + 6845013t^{80} + 5276926t^{81} + 4012238t^{82} + 3009500t^{83} + 2224150t^{84} \\
 & + 1620330t^{85} + 1161726t^{86} + 820356t^{87} + 569210t^{88} + 388723t^{89} + 260288t^{90} \\
 & + 171406t^{91} + 110398t^{92} + 69884t^{93} + 43083t^{94} + 26146t^{95} + 15342t^{96} + 8888t^{97} \\
 & + 4937t^{98} + 2723t^{99} + 1412t^{100} + 752t^{101} + 357t^{102} + 185t^{103} + 80t^{104} + 42t^{105} \\
 & + 16t^{106} + 11t^{107} + 3t^{108} + t^{109} + t^{113}.
 \end{aligned} \tag{A.1}$$

The numerator $R(t)$ of the rational Molien function in (111) is:

$$\begin{aligned}
R(t) = & 1 - t^4 + 3t^5 + 3t^6 + 4t^7 + 10t^8 + 12t^9 + 17t^{10} + 25t^{11} + 30t^{12} + 36t^{13} \\
& + 41t^{14} + 41t^{15} + 40t^{16} + 36t^{17} + 16t^{18} - 9t^{19} - 32t^{20} - 74t^{21} - 122t^{22} \\
& - 168t^{23} - 223t^{24} - 266t^{25} - 298t^{26} - 324t^{27} - 312t^{28} - 274t^{29} - 216t^{30} \\
& - 108t^{31} + 30t^{32} + 183t^{33} + 364t^{34} + 546t^{35} + 717t^{36} + 871t^{37} + 961t^{38} \\
& + 999t^{39} + 979t^{40} + 859t^{41} + 670t^{42} + 413t^{43} + 83t^{44} - 268t^{45} - 639t^{46} \\
& - 1002t^{47} - 1299t^{48} - 1536t^{49} - 1683t^{50} - 1695t^{51} - 1601t^{52} - 1398t^{53} \\
& - 1072t^{54} - 680t^{55} - 238t^{56} + 238t^{57} + 680t^{58} + 1072t^{59} + 1398t^{60} + 1601t^{61} \\
& + 1695t^{62} + 1683t^{63} + 1536t^{64} + 1299t^{65} + 1002t^{66} + 639t^{67} + 268t^{68} - 83t^{69} \\
& - 413t^{70} - 670t^{71} - 859t^{72} - 979t^{73} - 999t^{74} - 961t^{75} - 871t^{76} - 717t^{77} \\
& - 546t^{78} - 364t^{79} - 183t^{80} - 30t^{81} + 108t^{82} + 216t^{83} + 274t^{84} + 312t^{85} \\
& + 324t^{86} + 298t^{87} + 266t^{88} + 223t^{89} + 168t^{90} + 122t^{91} + 74t^{92} + 32t^{93} \\
& + 9t^{94} - 16t^{95} - 36t^{96} - 40t^{97} - 41t^{98} - 41t^{99} - 36t^{100} - 30t^{101} - 25t^{102} \\
& - 17t^{103} - 12t^{104} - 10t^{105} - 4t^{106} - 3t^{107} - 3t^{108} + t^{109} - t^{113}.
\end{aligned} \tag{A.2}$$

Appendix B. Quartic invariants

To understand the various relations among the invariant quantities, it is helpful to study the symmetries of the $U_{kk'}^{(j,j')}$ as defined in (131) which arise as a consequence of the symmetries of the $3j$ -symbols. In particular, we make use of the following identities [19]

$$\begin{aligned}
\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix} \\
\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix}
\end{aligned} \tag{B.1}$$

$$= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} \tag{B.2}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{B.3}$$

We now show that the relations among the invariants as given in equations (134b)–(134c) are simple consequences of the symmetries (B.1)–(B.3):

(i)

$$\begin{aligned}
U_{kk'}^{(j,j')} &= (-1)^{j+j'} \sum_{\substack{|m_i| \leq j \\ |m_i'| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ m_2 & m_1 & k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ m_2' & m_1' & k' \end{pmatrix} S_{m_2 m_2'} S_{m_1 m_1'} \\
&= (-1)^{j+j'} U_{kk'}^{(j,j')}.
\end{aligned} \tag{B.4}$$

Therefore, $U_{kk'}^{(j,j')} = 0$ if $j + j'$ is odd, and so is the associated invariant.

(ii)

$$\begin{aligned}
U_{kk'}^{(j,j')} &= (-1)^{j+j'} \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ -m_1 & -m_2 & -k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ -m'_1 & -m'_2 & -k' \end{pmatrix} S_{m_1 m'_1} S_{m_2 m'_2} \\
&= (-1)^{j+j'} \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ -m_1 & -m_2 & -k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ -m'_1 & -m'_2 & -k' \end{pmatrix} \\
&\quad \times (-1)^{m_1+m'_1+m_2+m'_2} S_{-m_1-m'_1}^* S_{-m_2-m'_2}^* \\
&= (-1)^{j+j'+k+k'} \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ -m_1 & -m_2 & -k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ -m'_1 & -m'_2 & -k' \end{pmatrix} \\
&\quad \times S_{-m_1-m'_1}^* S_{-m_2-m'_2}^* \\
&= (-1)^{j+j'+k+k'} \left(U_{-k, -k'}^{(j,j')} \right)^*. \tag{B.5}
\end{aligned}$$

Since we know from (i) that $j + j'$ must be even for non-vanishing U , we are left with

$$\left(U_{kk'}^{(j,j')} \right)^* = (-1)^{k+k'} U_{-k, -k'}^{(j,j')}. \tag{B.6}$$

This has the immediate consequence from (132) that the invariants $I_4^{(j,j')}$ are all real.

(iii) Finally, let us study how the $U_{kk'}^{(j,j')}$ transform under transposition,

$$\begin{aligned}
(\tau U^{(j,j')})_{kk'} &= \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j \\ m_1 & m_2 & k \end{pmatrix} \begin{pmatrix} 2 & 2 & j' \\ m'_1 & m'_2 & k' \end{pmatrix} \\
&\quad \times (-1)^{m_1+m'_1+m_2+m'_2} S_{-m'_1, -m_1} S_{-m'_2, -m_2} \\
&= (-1)^{k+k'} \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j' \\ -m'_1 & -m'_2 & k' \end{pmatrix} \begin{pmatrix} 2 & 2 & j \\ -m_1 & -m_2 & k \end{pmatrix} S_{m'_1 m_1} S_{m'_2 m_2} \\
&= (-1)^{k+k'+j+j'} \sum_{\substack{|m_i| \leq j \\ |m'_i| \leq j'}} \begin{pmatrix} 2 & 2 & j' \\ m'_1 & m'_2 & -k' \end{pmatrix} \begin{pmatrix} 2 & 2 & j \\ m_1 & m_2 & -k \end{pmatrix} S_{m'_1 m_1} S_{m'_2 m_2} \\
&= (-1)^{k+k'+j+j'} U_{-k', -k}^{(j',j)}. \tag{B.7}
\end{aligned}$$

From this we obtain

$$\tau I_4^{(j,j')} = \sum_{\substack{|k| \leq j \\ |k'| \leq j'}} (-1)^{k+k'} U_{-k', -k}^{(j',j)} U_{k', k}^{(j,j')} = I_4^{(j',j)}. \tag{B.8}$$

Therefore, the ‘diagonal’ invariants ($j = j'$) are left unchanged by the transposition. The ‘non-diagonal’ invariants ($j \neq j'$), in principle, are not. In terms of the symmetric and anti-symmetric parts of $I_4^{(j,j')}$, equation (B.8) yields

$$\tau I_4^{[j,j']} = I_4^{[j,j]}, \quad \tau I_4^{\{j,j'\}} = -I_4^{\{j,j'\}}. \tag{B.9}$$

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