The 3-dimensional Cycle Index of the Leapfrog of a Polyhedron

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Abstract

Relations between the 3-dimensional cycle index of the point group of a trivalent polyhedron or of a deltahedron on the one hand and of its leapfrog on the other hand are described.

The Leapfrog transformation is a method first invented for the construction of a fullerene $C_{3n}$ from a parent $C_n$ having the same as or even a bigger symmetry group than $C_n$. It was introduced by P.W. Fowler in his papers [2, 5]. (Molecules in the form of 3-connected polyhedral cages with exactly 12 pentagonal and all the other hexagonal faces solely built from carbon atoms are called fullerenes. Fullerenes $C_n$ can be constructed for $n = 20$ and for all even $n \geq 24$. They have $n$ vertices (i.e. C-atoms), $3n/2$ edges and $(n - 20)/2$ hexagonal faces. The most important member of the family of the fullerenes is $C_{60}$.)

In general the leapfrog transformation can be defined for any polyhedron $P$ as capping all the faces of $P$ and switching to the dual of the result. The leapfrog $L(P)$ is always a trivalent polyhedron having $2e_P$ vertices, $v_P + f_P$ faces and $3e_P$ edges, where $v_P$, $f_P$ and $e_P$ are the numbers of vertices, faces and edges of the parent $P$. When starting from a trivalent parent, the leapfrog has always $3v_P$ vertices.

In [6] it is described how the symmetry group of a fullerene $C_n$ (especially for $n = 20, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 70, 80$ and $140$) acts on its sets of vertices, faces and edges. Then general techniques from the theory of enumeration under finite group actions [7] are applied for determining the number of isomers of these molecules, or in other words for counting all the essentially different colourings of $C_n$. (Two colourings are called essentially different if they lie in different orbits of the symmetry group of $C_n$ acting on the set of all colourings of $C_n$.) Especially a 3-dimensional cycle index for the simultaneous action of the symmetry group on the sets of vertices, edges and faces of $C_n$ is presented.

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Whenever a group $G$ is acting on sets $X_1, \ldots, X_n$ then $G$ acts in a natural way on the disjoint union

$$X := \bigcup_{i=1}^{n} X_i.$$ 

The $n$-dimensional cycle index which uses for each set $X_i$ a separate family of indeterminates $x_{i,1}, x_{i,2}, \ldots$ is given by

$$Z_n(G, X_1 \cup \ldots \cup X_n) := \frac{1}{|G|} \sum_{g \in G} \prod_{i=1}^{n} \prod_{j=1}^{|X_i|} x_{i,j}^{a_{i,j}(g)},$$

where $(a_{i,1}(g), \ldots, a_{i,|X_i|}(g))$ is the cycle type of the permutation corresponding to $g$ and to the action of $g$ on $X_i$. (I.e. the induced permutation on $X_i$ decomposes into $a_{i,j}$ disjoint cycles of length $j$ for $j = 1, \ldots, |X_i|$.) For the action on the sets of vertices, edges and faces we usually denote the indeterminates by $v_i, e_i$ and $f_i$. Using the $n$-dimensional cycle index it is possible to determine the number of essentially different simultaneous colourings of $X_1 \cup \ldots \cup X_n$ as described in [6].

For instance the 3-dimensional cycle index for the action of the octahedral group $O_h$ acting on the cube is given by

$$Z_3(O_h, \text{cube}) = \frac{1}{48} \left( v_6^6 e_1^2 f_1^6 + 8v_4^4 e_3^2 v_3^2 f_2^3 + 6v_2^2 e_1^3 e_2^3 f_2^3 + 3v_3^4 e_2^5 f_1^3 f_2^2 + 6v_2^4 e_1^3 f_1^4 f_4 + 6v_1^4 e_2^3 e_1^3 f_1^4 f_2^2 + v_2^6 e_2^6 f_2^3 + 3v_2^4 e_1^4 f_1^4 f_2^2 + 8v_2^6 e_6^2 f_6 + 6v_2^2 e_3^5 f_2 f_4 \right).$$

These cycle indices are the basic tools for applying PÓLYA-theory [8] to the isomer count. It was already mentioned in [6] that the cycle types for the action on the set of faces of the leapfrog can easily be obtained from the 3-dimensional cycle index of the action on the parent. But for the actions on the sets of vertices and edges of the leapfrog we did not give satisfying methods.

Using the notation of spherical shell techniques the permutation representations for the actions on the sets of vertices, edges or faces of a polyhedron correspond to the so-called $\sigma$ representations. In [3, 4] it is shown how the $\sigma$ representations $\Gamma_{\sigma}(v, L)$, $\Gamma_{\sigma}(e, L)$ and $\Gamma_{\sigma}(f, L)$ for the actions on the components of the leapfrog $L = L(P)$ of an arbitrary polyhedron $P$ are related to the $\sigma$ representations $\Gamma_{\sigma}(v, P)$, $\Gamma_{\sigma}(e, P)$ and $\Gamma_{\sigma}(f, P)$ corresponding to the parent:

$$\Gamma_{\sigma}(f, L) = \Gamma_{\sigma}(v, P) + \Gamma_{\sigma}(f, P)$$

$$\Gamma_{\sigma}(v, L) = \Gamma_{\sigma}(e, P) + \Gamma_{\sigma}(f, P) + \Gamma_{\sigma}(v, P) \times \Gamma_{\sigma} - (\Gamma_0 + \Gamma_\varepsilon)$$

$$\Gamma_{\sigma}(e, L) = \Gamma_{\sigma}(f, L) \times \Gamma_\varepsilon - (\Gamma_T + \Gamma_R)$$

where $\Gamma_0$ is the totally symmetric representation with character $\chi_0(g) = 1$ for all $g$. The character of the antisymmetric representation $\Gamma_\varepsilon$ is $+1$ for all proper rotations and $-1$ for all improper rotations. $\Gamma_T$ (or $\Gamma_{xyz}$) is the translational representation, which is the
representation of a set of cartesian unit vectors at the origin, and $\Gamma_R = \Gamma_T \times \Gamma_\epsilon$ is the rotational representation.

These formulae can be rewritten in order to get the permutation characters for all $g$ in the symmetry group $G$ of $P$ by

$$\chi_{f,L}(g) = \chi_{v,P}(g) + \chi_{f,P}(g)$$

$$\chi_{e,L}(g) = \chi_{e,P}(g) + \chi_{f,P}(g) + \chi_{v,P}(g)\chi_\epsilon(g) - (1 + \chi_\epsilon(g))$$

$$\chi_{e,L}(g) = \chi_{f,L}(g)\chi_T(g) - (\chi_T(g) + \chi_\epsilon(g))$$

So far the permutation characters for the action on the components of the leapfrog are expressed in the permutation characters for the action on the components of the parent and in $\chi_\epsilon$ and $\chi_T$. Since usually the cycle indices both of the group of all symmetries and of the subgroup of all rotational symmetries of the parent are known we can assume that the antisymmetric character is known. Only for applying formula (6) we furthermore have to compute the translational character. In some cases however all the necessary information for computing $\chi_T$ is given by the 3-dimensional cycle index for the action on the parent $P$.

For instance if $P$ is a trivalent polyhedron (see [1]), then

$$\Gamma_\sigma(e, P) = \Gamma_\sigma(f, P) \times \Gamma_T - (\Gamma_T + \Gamma_R).$$

Combining (1) and (7) formula (3) can be written as

$$\Gamma_\sigma(e, L) = (\Gamma_\sigma(v, P) + \Gamma_\sigma(f, P)) \times \Gamma_T - (\Gamma_T + \Gamma_R)$$

$$\Gamma_\sigma(v, P) \times \Gamma_T = \Gamma_\parallel(e, P) + \Gamma_\sigma(e, P).$$

From [1] we deduce that

$$\Gamma_\sigma(v, P) \times \Gamma_T = \Gamma_\parallel(e, P) + \Gamma_\sigma(e, P)$$

and

$$\Gamma_\parallel(e, P) = (\Gamma_\sigma(f, P) - \Gamma_0) \times \Gamma_\epsilon + (\Gamma_\sigma(v, P) - \Gamma_0),$$

where $\Gamma_\parallel$ is the parallel representation. So finally (3) can be replaced by

$$\Gamma_\sigma(e, L) = (\Gamma_\sigma(f, P) - \Gamma_0) \times \Gamma_\epsilon + (\Gamma_\sigma(v, P) - \Gamma_0) + \Gamma_\sigma(e, P) + \Gamma_\sigma(e, P)$$

and the permutation character $\chi_{e,L}(g)$ can be computed as

$$\chi_{e,L}(g) = 2\chi_{e,P}(g) + (\chi_{f,P}(g) - 1)\chi_\epsilon(g) + (\chi_{v,P}(g) - 1).$$

If $P$ is a deltahedron, which is the dual of a trivalent polyhedron, then (6) can be replaced by

$$\chi_{e,L}(g) = 2\chi_{e,P}(g) + (\chi_{v,P}(g) - 1)\chi_\epsilon(g) + (\chi_{f,P}(g) - 1).$$
Using standard methods [7] the cycle type of \( g \in G \) can be computed from the permutation character of \( g \) and vice versa by

\[
a_k(g) = \sum_{d|k} \mu(k/d) a_1(g^d) \quad a_1(g^k) = \sum_{d|k} a_d(g),
\]

(10)

where \( \mu \) is the classical Möbius function.

Given a trivalent polyhedron or a deltahedron \( P \) with symmetry group \( G \) and subgroup \( H \) of rotational symmetries. Then the 3-dimensional cycle indices for the actions of \( G \) and \( H \) on the leapfrog \( L(P) \) can be computed from the 3-dimensional cycle indices for the actions on the parent \( P \) described above. It is worth to mention once more that no further group characters must be computed. In other words the 3-dimensional cycle indices for the action on the parent provide all the necessary information.

For example the cycle index for the leapfrog of the cube can be computed as:

\[
Z_3(O_h, L) = \frac{1}{48} \left( v_1^{24} e_1^{36} f_1^{14} + 8v_2^8 e_1^{12} f_1^2 f_4^4 + 6v_2^6 e_1^2 e_2^{17} f_2^7 + 3v_2^2 e_2^{18} f_2^2 f_6^6 + 6v_2^6 e_4 f_2^3 + 6v_2^6 e_1^2 f_6^4 + 6v_2^6 e_1^2 f_6^4 + 3v_1^2 v_2^6 e_1^2 e_2^{12} f_1^4 f_2^5 + 8v_6^6 e_6 f_2^3 + 6v_4^6 e_4 f_4^3 \right).
\]

In order to give another example we realize that \( C_{60} \) is the leapfrog of \( C_{20} \). They both are of icosahedral symmetry \( I_h \), the subgroup of all proper rotations will be denoted by \( I \). In [6] the following 3-dimensional cycle indices for the actions on the components of \( C_{20} \) can be found.

\[
Z_3(I, C_{20}) = \frac{1}{60} \left( v_1^{20} e_1^{30} f_1^{12} + 20v_2^2 e_1^6 f_3^3 + 15v_2^2 e_2^{14} f_6^6 + 24v_2^2 e_6 f_2^2 f_4^2 \right)
\]

\[
Z_3(I_h, C_{20}) = \frac{1}{2} Z_3(I, C_{20}) + \frac{1}{120} \left( v_2^{10} e_2^{15} f_2^6 + 20v_2^3 e_6 f_6^6 + 15v_1^4 e_1^8 e_2^{13} f_1^4 f_2^4 + 24v_2^2 e_3^3 f_2 f_6 \right).
\]

Applying (4), (5), (8) and (10) we compute:

\[
Z_3(I, C_{60}) = \frac{1}{60} \left( v_1^{60} e_1^{90} f_1^{32} + 20v_2^{40} e_3^{30} f_1^2 f_3^{10} + 15v_2^{30} e_1^4 e_2^{16} f_6^6 + 24v_2^{10} e_5 f_2^2 f_6^2 \right)
\]

and

\[
Z_3(I_h, C_{60}) = \frac{1}{2} Z_3(I, C_{60}) + \frac{1}{120} \left( v_2^{30} e_2^{45} f_2^{16} + 20v_1^{16} e_5 f_2^2 f_6^5 + 15v_1^4 e_2^{28} e_3^4 f_1^4 f_2^{12} + 24v_1^{10} e_1^9 f_2 f_6^3 \right).
\]

Iterating the leapfrog method once more we derive the 3-dimensional cycle index of \( C_{180} \) as

\[
Z_3(I, C_{180}) = \frac{1}{60} \left( v_1^{180} e_1^{270} f_1^{92} + 20v_2^{60} e_9^{30} f_1^2 f_3^{30} + 15v_2^{90} e_1^2 e_2^{134} f_2^4 f_6^{46} + 24v_2^{54} e_5 f_2^2 f_6^2 f_1^{18} \right)
\]

and

\[
Z_3(I_h, C_{180}) = \frac{1}{2} Z_3(I, C_{180}) + \frac{1}{120} \left( v_2^{90} e_2^{135} f_2^{16} + 20v_2^{30} e_4 f_2 f_6^{15} + 15v_1^{12} e_2^{84} e_1^2 e_2^{129} f_1^2 f_2^{40} + 24v_1^{18} e_2^7 f_2 f_6^9 \right).
\]
In order to compute the number of essentially different colourings of $C_{3n}$ it is necessary to compute the 3-dimensional cycle index for the action on $C_{3n}$ and apply the methods described in [6]. Only for the determination of the number of different colourings of the faces of $C_{3n}$ with $k$ colours the 3-dimensional cycle index of $C_n$ will do the job in the following way. Replace all the indeterminates in this cycle index corresponding to the actions on the sets of vertices and faces of $C_n$ by $k$ and all the indeterminates corresponding to the action on the set of edges by 1, then the expansion of this cycle index gives the number of different colourings of the faces of $C_{3n}$. For example the number of essentially different simultaneous colourings of $C_{20}$ with 2 colours for the vertices, 1 colour for the edges and 2 colours for the faces is computed as

$$Z_3(C_{20}, \text{I}_h, \ v_i = 2, \ e_i = 1, \ f_i = 2) = 35\,931\,952,$$

which is the number of different colourings of the faces of $C_{60}$ with 2 colours (cf. [6]). It should be mentioned that this number is not the product of the numbers of different colourings of the vertices and faces of $C_{20}$ with 2 colours. (These two numbers are given as 9,436 and 82 respectively.)

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References


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