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

Harald Fripertinger*

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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

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

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

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

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 $X_1 \dot{\cup} \ldots \dot{\cup} X_n$ as described in [6].

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

$$\begin{aligned} Z_3(\mathrm{O_h}, \text{cube}) \; = \; & \frac{1}{48}\Big(v_1^8 e_1^{12} f_1^6 + 8 v_1^2 v_3^2 e_3^4 f_3^2 + 6 v_2^4 e_1^2 e_2^5 f_2^3 + 3 v_2^4 e_2^6 f_1^2 f_2^2 + 6 v_4^2 e_4^3 f_1^2 f_4 + \\ & 6 v_1^4 v_2^2 e_1^2 e_2^5 f_1^2 f_2^2 + v_2^4 e_2^6 f_2^3 + 3 v_2^4 e_1^4 e_2^4 f_1^4 f_2 + 8 v_2 v_6 e_6^2 f_6 + 6 v_4^2 e_4^3 f_2 f_4 \Big). \end{aligned}$$

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 σ *representations*. In [3, 4] it is shown how the σ 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 σ representations $\Gamma_\sigma(v, P)$, $\Gamma_\sigma(e, P)$ and $\Gamma_\sigma(f, P)$ corresponding to the parent:

$$\Gamma_\sigma(f, L) = \Gamma_\sigma(v, P) + \Gamma_\sigma(f, P) \tag{1}$$

$$\Gamma_\sigma(v, L) = \Gamma_\sigma(e, P) + \Gamma_\sigma(f, P) + \Gamma_\sigma(v, P) \times \Gamma_\epsilon - (\Gamma_0 + \Gamma_\epsilon) \tag{2}$$

$$\Gamma_\sigma(e, L) = \Gamma_\sigma(f, L) \times \Gamma_T - (\Gamma_T + \Gamma_R) \tag{3}$$

where Γ_0 is the *totally symmetric* representation with character $\chi_0(g) = 1$ for all g. The character of the *antisymmetric* representation Γ_ϵ is $+1$ for all *proper rotations* and -1 for all *improper rotations*. Γ_T (or Γ_{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

$$\chi_{f,L}(g) = \chi_{v,P}(g) + \chi_{f,P}(g) \tag{4}$$

$$\chi_{v,L}(g) = \chi_{e,P}(g) + \chi_{f,P}(g) + \chi_{v,P}(g)\chi_\epsilon(g) - (1 + \chi_\epsilon(g)) \tag{5}$$

$$\chi_{e,L}(g) = \chi_{f,L}(g)\chi_T(g) - (\chi_T(g) + \chi_R(g)) \tag{6}$$

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 χ_ϵ and χ_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 χ_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

$$\Gamma_\sigma(e, P) = \Gamma_\sigma(f, P) \times \Gamma_T - (\Gamma_T + \Gamma_R). \tag{7}$$

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

$$\begin{aligned} \Gamma_\sigma(e, L) &= (\Gamma_\sigma(v, P) + \Gamma_\sigma(f, P)) \times \Gamma_T - (\Gamma_T + \Gamma_R) \\ &= \Gamma_\sigma(v, P) \times \Gamma_T + \Gamma_\sigma(e, P). \end{aligned}$$

From [1] we deduce that

$$\Gamma_\sigma(v, P) \times \Gamma_T = \Gamma_{||}(e, P) + \Gamma_\sigma(e, P)$$

and

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

where $\Gamma_{||}$ 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

$$\chi_{e,L}(g) = 2\chi_{e,P}(g) + (\chi_{f,P}(g) - 1)\chi_\epsilon(g) + (\chi_{v,P}(g) - 1). \tag{8}$$

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

$$\chi_{e,L}(g) = 2\chi_{e,P}(g) + (\chi_{v,P}(g) - 1)\chi_\epsilon(g) + (\chi_{f,P}(g) - 1). \tag{9}$$

Using standard methods [7] the cycle type of $g \in G$ can be computed from the permutation character of g and vice versa by

$$a_k(g) = \sum_{d|k} \mu(k/d) a_1(g^d) \qquad a_1(g^k) = \sum_{d|k} a_d(g), \tag{10}$$

where μ 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 as 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:

$$\begin{aligned} Z_3(\mathrm{O_h}, L) \;=\; & \frac{1}{48}\Big(v_1^{24}e_1^{36}f_1^{14} + 8v_3^8e_3^{12}f_1^2f_3^4 + 6v_2^{12}e_1^2e_2^{17}f_2^7 + 3v_2^{12}e_2^{18}f_1^2f_2^6 + 6v_4^6e_4^9f_1^2f_4^3 + \\ & 6v_2^{12}e_1^2e_2^{17}f_1^6f_2^4 + v_2^{12}e_2^{18}f_2^7 + 3v_1^8v_2^8e_1^{12}e_2^{12}f_1^4f_2^5 + 8v_6^4e_6^6f_2f_6^2 + 6v_4^6e_4^9f_2f_4^3\Big). \end{aligned}$$

In order to give another example we realize that C_{60} is the leapfrog of C_{20}. They both are of *icosahedral symmetry* $\mathrm{I_h}$, 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.

$$Z_3(\mathrm{I}, C_{20}) = \frac{1}{60}\left(v_1^{20}e_1^{30}f_1^{12} + 20v_1^2v_3^6e_3^{10}f_3^4 + 15v_2^{10}e_1^2e_2^{14}f_2^6 + 24v_5^4e_5^6f_1^2f_5^2\right)$$

$$Z_3(\mathrm{I_h}, C_{20}) = \frac{1}{2}Z_3(\mathrm{I}, C_{20}) + \frac{1}{120}\Big(v_2^{10}e_2^{15}f_2^6 + 20v_2v_6^3e_6^5f_6^2 + 15v_1^4v_2^8e_1^4e_2^{13}f_1^4f_2^4 + 24v_{10}^2e_{10}^3f_2f_{10}\Big).$$

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

$$Z_3(\mathrm{I}, C_{60}) = \frac{1}{60}\left(v_1^{60}e_1^{90}f_1^{32} + 20v_3^{20}e_3^{30}f_1^2f_3^{10} + 15v_2^{30}e_1^2e_2^{44}f_2^{16} + 24v_5^{12}e_5^{18}f_1^2f_5^6\right)$$

and

$$\begin{aligned} Z_3(\mathrm{I_h}, C_{60}) = \frac{1}{2}Z_3(\mathrm{I}, C_{60}) + \quad \frac{1}{120}\Big(\quad & v_2^{30}e_2^{45}f_2^{16} + 20v_6^{10}e_6^{15}f_2f_6^5 + \\ & 15v_1^4v_2^{28}e_1^8e_2^{41}f_1^8f_2^{12} + 24v_{10}^6e_{10}^9f_2f_{10}^3\Big). \end{aligned}$$

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

$$Z_3(\mathrm{I}, C_{180}) = \frac{1}{60}\left(v_1^{180}e_1^{270}f_1^{92} + 20v_3^{60}e_3^{90}f_1^2f_3^{30} + 15v_2^{90}e_1^2e_2^{134}f_2^{46} + 24v_5^{36}e_5^{54}f_1^2f_5^{18}\right)$$

and

$$\begin{aligned} Z_3(\mathrm{I_h}, C_{180}) = \frac{1}{2}Z_3(\mathrm{I}, C_{180}) + \quad \frac{1}{120}\Big(\quad & v_2^{90}e_2^{135}f_2^{46} + 20v_6^{30}e_6^{45}f_2f_6^{15} + \\ & 15v_1^{12}v_2^{84}e_1^{12}e_2^{129}f_1^{12}f_2^{40} + 24v_{10}^{18}e_{10}^{27}f_2f_{10}^9\Big). \end{aligned}$$

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

$$Z_3(\mathrm{C}_{20}, \mathrm{I_h},\ v_i = 2,\ e_i = 1,\ f_i = 2) = 35\,931\,952,$$

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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Address of the author:
HARALD FRIPERTINGER
Institut für Mathematik
Karl-Franzens-Universität Graz
Heinrichstr. 36
A-8010 Graz
e-mail: `harald.fripertinger@kfunigraz.ac.at`