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Application of Group Ring Type Structure in Chemistry

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Abstract

In this paper we have described about the algebraic structure Burnside Ring and produces an application by giving an example in chemistry as the labeling of atoms in molecules of high symmetry. Also we have discussed on the construction of symmetry adapted functions. For showing such applications, we have applied the concept of Burnside ring to the icosahedral symmetry. As an example we have taken an equilateral triangle in this research paper. But we may choose other example too such as regular triangular prism etc. We may use the Burnside ring as group ring structure also in some what extent. $B(G) = \{\sum_1^n a_i({}^{G}/_{G_i}) : a_i \in Z\}$. This algebraic structure is looking like analogous to group ring structure $R[G] = \sum_{g \in G}^n a_g g : a_g \in R$. So we have suggested Burnside ring as a special case group ring structure.

Key words: Burnside ring, icosahedral symmetry, symmetry adapted functions, Burnside matrix, quotient group, subgroup, Burnside lemma, symmetric group,

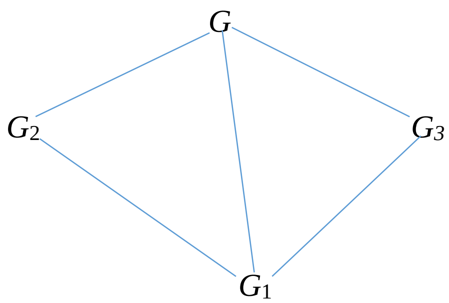
1.Introduction

Burnside idea have been applied to algebra of ring structure. We will define the Burnside ring $B(G)$ of the group G as follow, $B(G) = \{ \sum_1^n a_i ({}^{G}/_{G_i}) : a_i \in Z \}$. Burnside ring is commutative ring with the identity ${}^{G}/_{G_n}$ here, any sum$({}^{G}/_{G_i}) + ({}^{G}/_{G_j})$ is the disjoint union of ${}^{G}/_{G_i}$ and ${}^{G}/_{G_j}$ aa well as the product $({}^{G}/_{G_i}) \times ({}^{G}/_{G_j})$ is the cartesian product of ${}^{G}/_{G_i}$ and ${}^{G}/_{G_j}$, this means, Z is the set of integer. Now we understand Burnside's lemma. For this we will define a group action. If G be a group and X be any set then a left group action of G on X is a binary function such that $G \times X \rightarrow X$ or we have $(g, x) \mapsto gx$. This group action binary function is based on two rules, **(*i*).** $(gh).x = g.(hx)\ \forall\ g, h \in G$ and $\forall\ x \in G$. **(*ii*).** $ex = x$ for every x in X. Here e is identity element of group G. Now we define an orbit on group action of G on X. Further we define orbit. Let us consider G be a group and functioning on X. Let x be element of X, then orbit of x is denoted by Gx. We can write $Gx = \{g.x \mid g \in G\}$. Thus gx is element of X, which shows that x moves by g in X. For each g in G we suppose X^g be the set of fixed points in X. So we have Burnside's lemma as, $|X/G| = \frac{1}{|G|}\sum_{g\in G}|X^g|$. Let us suppose that $\boldsymbol{\Omega} = \{G=1, G_2, G_3, \ldots\ldots\ldots, G_s = G\}$ be a full set of nonconjugated subgroups of G. The set of transitive G-sets $\{{}^{G}/_{G_i}: i = 1, 2, \ldots\ldots, n\}$ will be a complete set of orbits. This means every G-set S is isomorphic to a disjoint union of such each orbits. $S \cong \bigcup_i^n a_i({}^{G}/_{G_i})$. The coefficients a_i are uniquely determined and can be computed as the system of linear equations, $\sum_{i=1}^n M_{ij}\, a_j = b_j$ $j = 1, 2, 3\ldots\ldots.., n$. Thus, $a_i = \sum_{j=1}^n M^{-1}{}_{ij}\, b_j$ $i = 1, 2, 3, \ldots\ldots., n$. Here, M^{-1} is known as Burnside matrix.

Let us suppose that G be a finite group. Two G sets are S and T. Then action of G on $S \times T$ will be given as $g(x, y) = (g(x), g(y))$ for any $g \in G$ and $(x, y) \in S \times T$ as well as $S \times T$ is a G-set. Now the Cartesian product of the G-sets ${}^{G}/_{G_i}$, ${}^{G}/_{G_j}$ is a G-set, then it is isomorphic to a disjoint union of orbits. ${}^{G}/_{G_i} \times {}^{G}/_{G_J} \cong \bigcup_k^n n_{ij,k}({}^{G}/_{G_k})$. If G_l is subgroup of G then the number of fixed points of G_l in ${}^{G}/_{G_i}$ and ${}^{G}/_{G_j}$ will be M_{li} and M_{lj} respectively. So the number of fixed points of G_l in $({}^{G}/_{G_i}) \times ({}^{G}/_{G_j})$ will be $M_{li}M_{lj}$.Now we get, $n_{ij,k} = \sum_l (M^{-1})_{kl} M_{li} M_{lj}$. The Burnside ring $B(G)$ of the group G will be defined as, $B(G) = \{\sum_{i=1}^n a_i({}^{G}/_{G_i}): a_i \in Z\}$, Here Z is the set of integer numbers.

Let us suppose that G be a finite group and R be a ring, then set of all linear combinations in the form written as, $R[G] = \sum_{g\in G} a_g g$: $a_g \in R$. This group ring $R[G]$ algebraic structure may be regarded as analogous to that of Burnside ring $B(G)$

2. We produce an example of Burnside ring corresponding to symmetric group $\boldsymbol{S_3}$. We use to denote S_3 by G. Therefore $G = \{e, r, r^2, s, rs, r^2s\}$. Now we construct subgroups of G. $G_1 = \{e\}$, $G_2 = \{(e, s), (e, r^2s), (e, r^2s\}$, $G_3 = \{e, r, r^2\}$, $G_4 = \{e, r, s, rs, r^2s\}$. From these subgroups we construct the subgroup lattice of G, as follow,



Now we arrange a set of quotient group, $\{G/G_1, G/G_2, G/G_3, G/G_4\}$ with G/H = $\{Gh|g \in G\}$. So we have **(*i*).** $G/G_1 = \{\{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\}\}$ **(*ii*).** $G/G_2 = \{e, r, r^2\} \bullet \{e, s\} = \{\{e, s\}, \{r, rs\}, \{r^2, r^2s\}\}$ **(*iii*).** $G/G_3 = \{e, s\} \bullet \{e, r, r^2\} = \{\{e, r, r^2\}, \{s, rs, r^2s\}\}$ **(*iv*).** $G/G_4 = G/G = \{\{e, r, r^2, s, rs, r^2s\}\}$.

3.Marks, the simplification of the Burnside ring *B*(*G*) : Let us suppose that for a given group *G* acting on a set *X*, and *H* be subgroup of *G*, then the mark of *H* on *X* $m_x(H) = |X^H|$ here $|X^H| = \{ x \in X \mid h.x = x, \forall h \in H \}$. Therefore, the mark of a product $G_i \bullet (G/G_j)$ will be equal to total number of fixed points.

4. Number of fixed points for each group action:

(*i*) $G_1 \bullet (G/G_1)$ has 6 fixed points, **(*ii*)** $G_2 \bullet (G/G_1)$ has 0 fixed points **(*iii*)** $G_3(G/G_1)$ has 0 fixed point, **(*iv*)** $G_4 \bullet (G/G_1)$ has also 0 fixed point. Therefore, the first row of table will be [6, 0, 0, 0]. Similarly group action on G/G_2 will produce second row of mark table as [3, 1, 0, 0] also, third as well as fourth rows of mark table are [2, 0, 2, 0] and [1, 1, 1, 1]. We will produce a table of marks of 4×4 matrix *M*, which is given below,

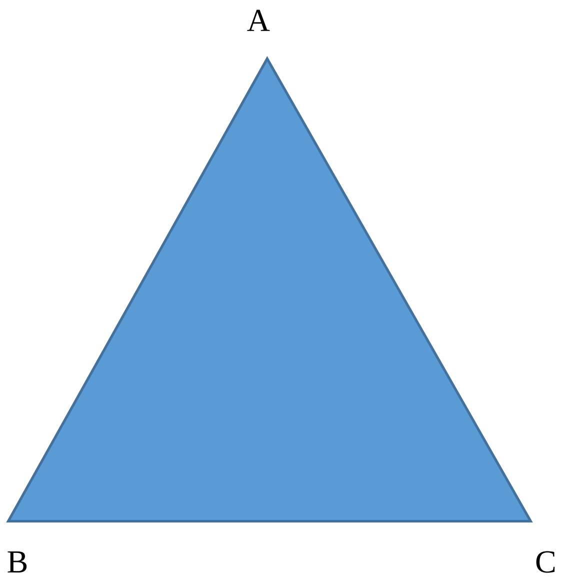
G	G/G_1	G/G_2	G/G_3	G/G_4
G_1	6	3	2	1
G_2	0	1	0	1
G_3	0	0	2	1
G_4	0	0	0	1

Now we obtain M^{-1} as follow,

$$M^{-1} = \begin{pmatrix} 1/6 & -1/2 & -1/6 & 1/2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1/2 & -1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

5. Equilateral triangle and icosahedral symmetry as well as the use of Burnside ring:

Now we consider an equilateral triangle as an example here and use the Burnside ring to show icosahedral symmetry. It is very simple example that will illustrate the use of Burnside ring in icosahedral symmetry.



We take set X as the set of all possible triangles. So we have observed that first vertex has 3 choices second has 2 choices while third has 1 choice. Therefore total number of triangles possible are $3 \times 2 \times 1 = 6$. Now we compute the coefficient a_i from the Burnside matrix for each coset G/G_i .

$a_i = \sum_{j=1}^{s} (M^{-1})_{ij}\, b_j$ here i= 1, 2, 3,……, s and b_j is number of elements in X which are fixed points to G_J. Now we get b_j by putting j = 1, 2, 3, ……, s.

$b_1 = 6$

$b_2 = 0$ Thus, $b_j = \begin{pmatrix} 6 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

$b_3 = 0$

$b_4 = 0$

Now we compute, $(M^{-1})_{ij} b_j = \begin{pmatrix} 1/6 & -1/2 & -1/6 & 1/2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1/2 & -1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 6 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

Now we find,
$a_i = \sum_{i=1}^{4} [1, 0, 0, 0] \bullet {}^{G}/_{G_I} = {}^{G}/_{G_1} = \{\{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2 s\}\}$. Thus each element of *G* generates one of the six possible equilateral triangle.

6. Conclusions

Burnside ring has analogous structure that of group ring algebraic structure. With the help of Burnside ring we have tried to show the action of symmetric group S_3 on the set of equilateral triangles. But we can apply S_3 acting on a larger set. Here, we have showed the labelling of molecules on the vertices of equilateral triangle. But it opens the way to apply this ring on complex geometric shapes such as regular triangular prism and much more. We have also seen that the Burnside ring helps to simplify and decompose the complex geometric structures and makes easier in labelling of molecules. As we know that $G = S_3$ on the set of equilateral triangle is an simple example, but no matter what the size of the group or the set on which the groups acts, the procedure of labelling and simplification of complex geometric shapes will remain same as applied on equilateral triangle. We have observed that for the set *X* its elements of the Burnside ring is the vector $[1, 0, 0, 0]^T$ also this set is congruent to $\sum_{i=1}^{4} [1, 0, 0, 0] \bullet {}^{G}/_{G_i} = \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2 s\} \}$. It is clear that each element of *G* generates one of the six possible equilateral triangles.

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