

# On the Partition Functions Induced by Iterated ( $k$ -Folded) Wreath Product Groups

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## Abstract

Group theory provides a systematic way of thinking about symmetry. Wreath products are group-theoretic constructions that have been used to model symmetries in a whole variety of research disciplines. The goal of this paper is to calculate the partition functions induced by these algebraic structures when organized iteratively under the symmetries imposed by the permutation and cyclic groups. The resulting hierarchical structures are modeled as Cayley-like trees from a statistical mechanics point of view, whereas the interactions between the nodes of those trees are defined by the actions induced by these groups. The emphasis is put on the analytic combinatorics treatment of the problem as a way to obtain closed expressions for the partition functions. Furthermore, the advantages of the singularity analysis and symbolic techniques of this mathematical theory are stressed as a way of extracting asymptotic information and setting up functional relations between partition functions.

**Keywords:** Group Theory, Statistical Mechanics, Analytic Combinatorics

## 1 Introduction

Symmetries are present in nature at all scales of complexity, from the atomic and molecular levels to the scale of big cosmological structures. The precise

notions of symmetry have various measures and operational definitions. For example, symmetry may be observed with respect to the passage of time, as a spatial relationship, through geometric transformations such as rotation, scaling, and reflection or through other kinds of functional transformations. From an historical perspective mathematical structures which generated symmetrical patterns were not systematically studied until the nineteenth century. With the advent of quantum mechanics and the standard model of elementary particle physics the importance of symmetries was reinforced and took a central role in the study on nature. Nowadays, symmetries underlie some of the most profound results found in modern physics, including aspects of space and time [19] or quantum mechanics [13].

From a mathematical point of view symmetries can be exploited to simplify the modeling of their physical properties. Group theory [2, 12, 11, 16, 15] provides a systematic way of thinking about symmetries. Wreath products are group theory constructions that have been extensively used in mathematics and physics [5] to model the physical properties of objects of different kind like molecular dynamics [8], coupled arrays of Josephson junctions [1], discretizations of partial differential equations with local gauge symmetry [7], or heteroclinic cycles [9] just to mention a few. Furthermore, more recently, this algebraic construction has been also used to describe highly complex shapes in computer-aided design, computer vision in robotics, assembly planning and machining between others within the context of a generative theory of shape [14].

Moreover, statistical mechanics [3, 17] is one of the active research disciplines in Physics where discrete probabilistic models are commonly used. Specifically, partition functions are the central mathematical object of study in this discipline. However, their analytic or exact calculation is often not possible because of the mathematical complexity. In this paper the partition functions induced by these algebraic constructions are calculated when they are used iteratively under the symmetries imposed by the permutation and cyclic groups. The resulting hierarchical structures are modeled as Cayley trees from a statistical mechanics point of view, whereas the interactions between the nodes of these structures are defined by the actions induced by these groups. The emphasis is put on the analytic combinatorics treatment of the problem as a way to obtain closed expressions for the partition functions. The analytic combinatorics treatment of the calculation leads to formulate partitions functions in terms of generating functions of energy.

The rest of the paper is organized as follows: In the next section wreath products are presented from a pure algebraic point of view. After defining wreath products, this construction is iterated as a way of modeling the symmetries of more complex structures. Section 3 discusses the problem of representation. In other words, how the iteration of this algebraic construction can

be expressed in terms of the language of statistical physics. More specifically, partition functions are expressed as generating functions of energies to facilitate their posterior combinatoric treatment. Sections 4 and 5 are devoted to illustrate the advantages of the analytic combinatorics formulation. Following the translation schema introduced in section 3, the partition functions induced by the permutation and cyclic groups symmetries are calculated analytically in sections 4 and 5 respectively. Furthermore, practical applications of the symbolic and the complex asymptotic methods derived from the theory are also presented. Finally, section 6 provides a summary of the present study and some concluding remarks.

## 2 Wreath Products

### 2.1 Definition and Group Structure

The wreath product operation on two finite groups  $G_2$  and  $G_1$ , with orders  $|G_2| = m_2$  and  $|G_1| = m_1$  respectively is denoted as  $G_2 \wr G_1$ . The information contained by this particular group construction is really the semi-direct prod-

uct (represented by the symbol  $\wr$ ) of the fiber-group product  $\overbrace{G_2 \otimes G_2 \otimes \cdots \otimes G_2}^{m_1 \text{ times}}$  (where the symbol  $\otimes$  indicates a direct product operation) and the group  $G_1$ . Both expressions are simply two different notations for the same group, although the semi-direct product notation reveals more of the structure of the wreath product:

$$G_2 \wr G_1 = \overbrace{[G_2 \otimes G_2 \otimes G_2 \otimes \cdots \otimes G_2]}^{m_1 \text{ times}} \wr G_1 \tag{1}$$

It is important to note that the semi-direct group operation describes an action

of the group  $G_1$  on the group  $\overbrace{G_2 \otimes G_2 \otimes \cdots \otimes G_2}^{m_1 \text{ times}}$ , that is, a function  $\phi$ :

$$\phi : G_1 \longrightarrow \text{Aut}(\overbrace{G_2 \otimes G_2 \otimes \cdots \otimes G_2}^{m_1 \text{ times}}) \tag{2}$$

which defines a mapping  $\phi$  of the group  $G_1$  in the automorphism of the direct product of  $m_1$  copies of group  $G_2$  representing the aforementioned group action.

The 2-fold wreath product operation of expression (1) can be represented graphically as a tree (see the left side of the graph of figure 1) of two levels (depth of the tree), where the level 2 of the tree is representing the copies of the fiber group  $G_2$  whereas, the level 1 (the root of the tree) is representing the group  $G_1$  denoted hereafter as the control group to emphasize the fact that this group is acting on the fiber group copies  $G_2 \otimes G_2 \otimes \cdots \otimes G_2$ . To add a

third group  $G_3$  (see the right side of the graph of figure 1), the operation is applied again, as follows:  $(G_3 \wr G_2) \wr G_1$ .

$$\begin{aligned}
 (G_3 \wr G_2) \wr G_1 &= \overbrace{[(G_3 \wr G_2) \otimes (G_3 \wr G_2) \otimes \cdots \otimes (G_3 \wr G_2)]}^{m_1 \text{ times}} \wedge G_1 = & (3) \\
 &= \overbrace{\left[ \overbrace{[G_3 \otimes \cdots \otimes G_3]}^{m_2 \text{ times}} \wedge G_2 \right] \otimes \cdots \otimes \left[ \overbrace{[G_3 \otimes \cdots \otimes G_3]}^{m_2 \text{ times}} \wedge G_2 \right]}^{m_1 \text{ times}} \wedge G_1
 \end{aligned}$$

The parentheses indicate that  $G_3 \wr G_2$  is a fiber group relative to the second wreath product symbol  $\wr$ , and  $G_1$  is the group (the control group) acting on that symbol (i.e., the group  $(G_3 \wr G_2)$ ). Therefore, the hierarchy of control ascends from left to right. More specifically, on the far left of equation (3), there is the fiber-group product  $G_3 \otimes G_3 \otimes \cdots \otimes G_3$ . This is the first level of fibers  $G_3$ . In particular, this product consists of  $m_2$  copies of  $G_3$  since there is one copy for each element in its immediate control group  $G_2$ . Progressing one step rightwards along the sequence, the symbol  $\wedge$  is found corresponding to the semi-direct product, which indicates that one level up in the hierarchy is reached, because the semi-direct product symbol  $\wedge$  is hierarchical. That is, following the  $\wedge$ , there is  $G_2$ . This completes the first hierarchy along the sequence, i.e.,  $[G_3 \otimes G_3 \otimes \cdots \otimes G_3] \wedge G_2$ . Now moving rightward along the sequence (3), it is evident that the hierarchy just given is actually copied a number of times. In fact, it is copied  $m_1$  times because there are  $m_1$  elements in the immediate control group  $G_1$ . Thus, the initial  $m_2$ -fold duplication of  $G_3$  is itself duplicated  $m_1$  times. In other words,  $G_3$  is duplicated  $m_1 \times m_2$  times.

### 2.2 Iterated Wreath Product

The group-theoretic construction associated to the wreath product can be iterated to obtain a generic  $k$ -fold wreath product of  $k$  levels, where  $k \geq 2$ . In the  $k$ -fold case, one gets:

$$(\cdots (((((G_k \wr G_{k-1}) \wr G_{k-2}) \wr G_{k-3}) \wr G_{k-4}) \wr \cdots) \wr G_2) \wr G_1 \tag{4}$$

It is important to understand that the  $k$ -fold wreath product is a group, and also that any group  $G_i$ , where  $1 \leq i \leq k$  along the  $k$ -fold sequence acts to its left, in fact, on the entire hierarchy to its left. This hierarchy is called the left-subsequence of  $G_i$ . The relation between  $G_i$  and its left subsequence is simply that between a control group and its fiber group. For instance, figure 2 graphically represents an iterated wreath product operation of  $k$  levels when the group components under consideration are action groups. The resulting graph is a Cayley-like tree structure where each of the nodes comprising the

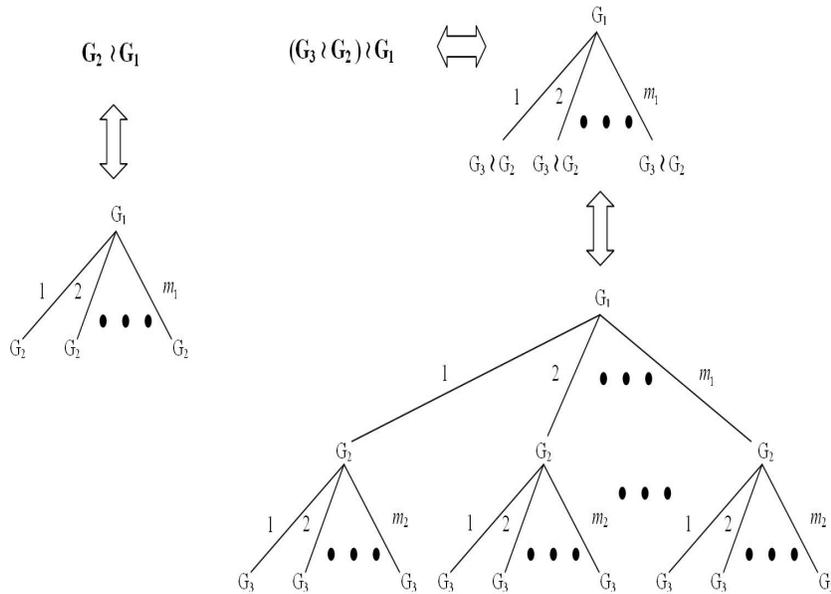


Figure 1: The left part of the figure provides a graphical interpretation of the wreath product group operation  $G_2 \wr G_1$ . Specifically, the first level of the structure represents the control group  $G_1$ , whereas the second level of the structure is representing the copies of the fiber group  $G_2$ . It is assumed that there are as many copies of  $G_2$  as there are elements within the group  $G_1$  on level 1. Note that  $G_1$  moves the copies of  $G_2$  around onto each other under the transfer automorphism. Similarly, the right part of the figure represents the 3-fold wreath product operation  $(G_3 \wr G_2) \wr G_1$ . In this case, the top part of the figure represents a structure of two levels. The wreath product  $G_3 \wr G_2$  has not been unfolded to show that the resulting group (i.e.,  $G_3 \wr G_2$ ) is acting as the fiber group of the wreath product operation with the group  $G_1$ , which is acting as the control group like in the two-fold situation depicted on the left part of the figure. The bottom of the figure illustrates the associated tree when the entire wreath product  $(G_3 \wr G_2) \wr G_1$  has been unfolded. At level 2, there are as many copies of the group  $G_2$  as elements in its immediate control group  $G_1$ , i.e.,  $m_1$  elements, whereas at level 3 (i.e., the bottom of the tree) there are  $m_1 \times m_2$  copies of the group  $G_3$ .

structure is representing a group. The root node of the structure corresponds to the group  $G_1$ , whereas the leaf nodes of the tree represent copies of the fiber group  $G_k$ . Furthermore, in the  $k$ -fold situation there are a set of copies of group  $G_i$  on level  $i$  that are connected to a single copy of  $G_{i-1}$  on the level  $i - 1$ . Furthermore, each node (excepting the root and the leaves nodes) acts both as a control group of the level immediately below and as a fiber group of the group immediately above. Two structural parameters define the aspect of these trees. Namely, the depth of the structures that represents the number of groups involved in the iterated wreath-product operation and the branching factor associated to each level that is in direct correspondence with the number of elements of the sets where the groups are acting (i.e.,  $m_i$ , for the action group  $G_i$ , where  $1 \leq i \leq k$ ). The circular arrows are used to illustrate the actions of the control groups over the fiber group copies.

Finally, it is important to mention that this kind of multilevel algebraic constructions have been extensively used in [14] to describe highly complex shapes in constructive solid geometry, architectural computer-aided design, robot manipulators, assembly planning and machining within the context of a generative theory of shape. This mathematical theory (mainly based in the iterated wreath product construction) characterizes the structure of any shape by a sequence of actions needed to generate it, in other words, a given data set is represented by a program that generates the set.

## 3 Problem Representation

### 3.1 Statistical Mechanics Formulation

From a statistical mechanics point of view, a natural way of modeling the hierarchical structures induced by iterated wreath product groups (see figures 1 and 2) is in terms of multi-state variables arranged hierarchically as it is shown in figure 3. Firstly, this figure corresponds to the modelization, from a statistical physics perspective, of the structure represented in figure 2. It is important to remember that the number of levels is in direct correspondence with the number of groups involved in the iterated wreath product operation, i.e.,  $k$  groups in this case (see equation (4)). The branching factor associated to each level is in direct correspondence with the number of elements of the set where the group is acting, i.e.,  $m_i$  for the group  $G_i$ , where  $1 \leq i \leq k$ . Furthermore, there are as many multi-state variables as nodes are in figure 2. It is important to emphasize that each node is representing a group, i.e., the fiber-group copies of the groups associated to each level of the tree, excepting the root node of the tree that represents the control group  $G_1$  situated on top of the hierarchy (the unique control group that is not also acting as a fiber group).

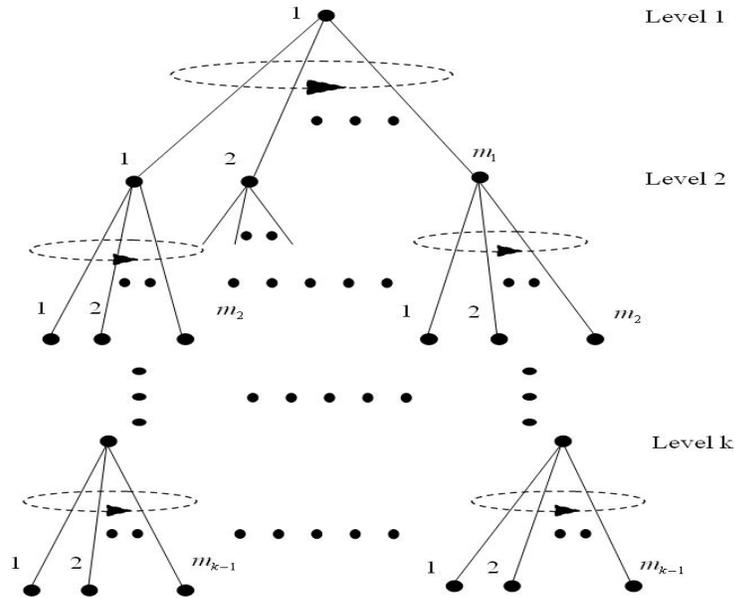


Figure 2: Graphical representation of an iterated wreath product operation of  $k$  levels (see equation (4) ) when the group components under consideration are action groups. The resulting graph is a Cayley-like tree structure where each of the nodes comprising the structure is representing a group. The root node of the structure corresponds to the group  $G_1$ , whereas the leaf nodes of the tree represent copies of the fiber group  $G_k$ . In the  $k$ -fold situation there are a set of copies of group  $G_i$  on level  $i$  that are connected to a single copy of  $G_{i-1}$  on the level  $i - 1$ . Furthermore, each node (excepting the root and the leaves nodes) acts both as a control group (i.e., an action group) of the level immediately below and as a fiber group of the group immediately above. Two structural parameters define the aspect of these trees. Namely, the depth of the structures that represents the number of groups involved in the iterated wreath-product operation and the branching factor associated to each of the levels of the structure that represents the number of elements of the sets where the groups are acting (i.e.,  $m_i$  elements for the group  $G_i$ , where  $1 \leq i \leq k$ ). The circular arrows are used to illustrate the action of the control groups over the fiber group copies.

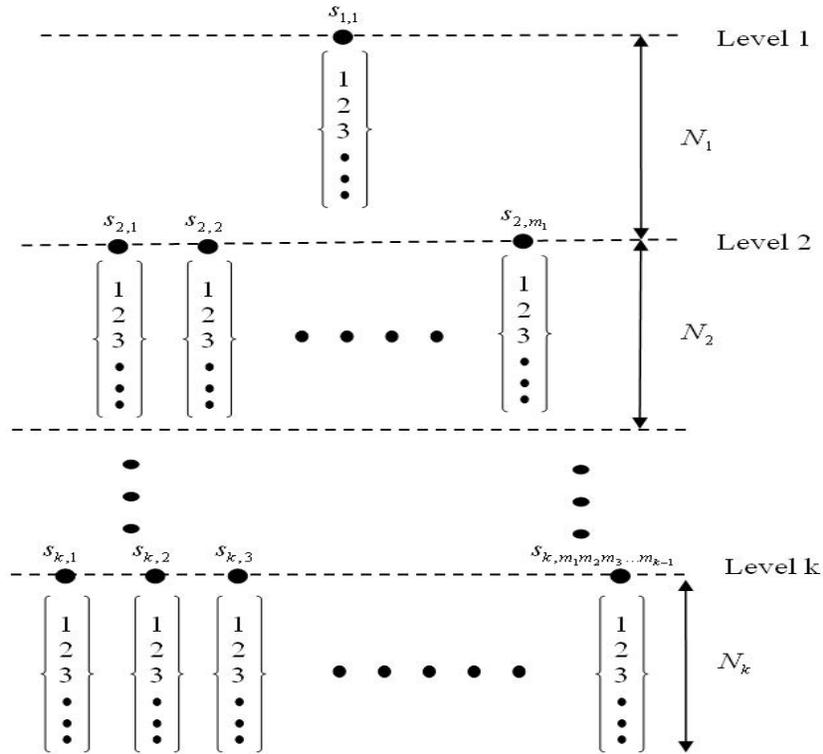


Figure 3: Graphic illustration of the modelization of the iterated ( $k$ -fold) wreath product operation corresponding to equation (4) from a statistical physics perspective. The structure of algebraic connectivity associated to this operation (see figure 2) is mapped to a hierarchy of multi-state variables. The number of levels is in direct correspondence with the number of groups involved in the iterated wreath product operation, i.e.,  $k$  groups. Each level is represented by a certain number of variables  $s_{i,j}$ , where  $1 \leq i \leq k$  and  $1 \leq j \leq m_1 m_2 m_3 \dots m_{k-1}$  that can be in a finite number of states (indicated within curly brackets). The number of variables is in direct correspondence with the fiber-group copies of the groups associated to each level of the tree (see figures 1 and 2). The cardinality of the local energy values associated to the multi-state variables depends on the energy model used, which exploits the particularities associated to the action groups. The variables  $N_i$ , where  $1 \leq i \leq k$  are employed to describe the energy values associated to each level of the structure (i.e., combinatorial classes in the language of analytic combinatorics).

Secondly, each level is represented by a certain number of variables  $s_{i,j}$ , where  $1 \leq i \leq k$  and  $1 \leq j \leq m_1 m_2 m_3 \cdots m_{k-1}$  that can be in a finite number of states (indicated within curly brackets) representing one of the possible local energy values. Each particular configuration of the elements of the set, as a result of a group action, leads to a specific energy value represented by one of the states of the multi-state variables. The energy function (i.e., the Hamiltonian) is defined in terms of a cost function (yet to be defined precisely) that computes a distance of local configurations of nodes (represented by the elements of the groups) with respect to a resting state configuration. The resting state configuration is always represented by the identity member of the groups. Each state is represented by an integer value which indicates its energy cost. The higher the energy of the state, the higher its energy value (i.e., the associated integer value). The resting state always has an energy value equal to 1. The variables  $N_i$ , where  $1 \leq i \leq k$  that appear on the right part of the graph are used to describe, in the following sections, the energy values associated to each level of the structure (i.e., combinatorial classes). Finally, the cardinality of the set of states depends on the energy model used although is related to the branching factor of the level where the multi-state variable belongs. Specifically, the aforementioned cardinality is related to the particularities of the action group.

In the following sections it is assumed that each of the group components  $G_i$  comprising the aforementioned structure of  $k$ -levels are finite and acting on a set  $\Omega_m = \{c_1, c_2, c_3, \cdots, c_m\}$ , where  $m$  is an integer value. In other words, it is assumed that each group  $G_i$  (where  $1 \leq i \leq k$ ) comprising the hierarchy is an action group. A group action is defined as a group homomorphism  $\tau$  from  $G_i$  to the symmetric group on  $\Omega_m$ . The action assigns a permutation of  $\Omega_m$  to each element of the group in such a way that the permutations of  $\Omega_m$  assigned to the identity element of  $G_i$  is the identity transformation of  $\Omega$  (the fixed point permutation  $c_1 c_2 c_3 \cdots c_m$ ). Similarly, a product of two elements  $g_1$  and  $g_2$  such as  $g_1, g_2 \in G_i$  is the composition of the permutations assigned to  $g_1$  and  $g_2$ . It is important to emphasize that a group action is also known as a permutation representation [2, 12]. The particular mapping between configurations of the elements and local energy values (i.e., the states of the multi-state variables) is further specified in sections 4 and 5.

### 3.2 The Energy Model: General Considerations

The main idea in statistical mechanics [3, 17] is that every microscopic configuration  $C$ , (e.g. the particle's positions, spin orientations or the configurations of the elements of the sets where the groups are acting in our case) is assigned a probability  $p(C)$  which depends on its energy  $H(C)$  and is given by the Boltzmann-Gibbs distribution. The partition function is defined as the nor-

malization factor of the distribution and it can be interpreted as a generating function of energies [10]:

$$Z = \sum_C e^{-\beta H(C)} = \sum_n N(n) e^{-\beta n} \quad (5)$$

In the previous expression  $\beta$  is equal to the inverse of the temperature  $T$  and  $N(n)$  is the number of configurations  $C$  having exactly energy equal to  $n$ , i.e.,  $n = H(C)$ . Here the Hamiltonian  $H(C)$  is defined in terms of the particular arrangement of the elements of the sets where the groups (i.e., the nodes of the Cayley-like structures) are acting. More specifically, as a function of the states associated to the multi-state variables.

The mechanism of assignment of configurations to multi-state local energy values is based on the idea that moving the system away from its resting state has an associated energy cost. Configurations are defined as any particular arrangement of the elements belonging to the sets  $\Omega_m$  as a result of the group actions (i.e., the groups comprising the  $k$ -fold wreath product operation). The higher the energy of the state, the higher its energy value (i.e., the associated integer value). The resting state always has an energy value equal to 1 that represents the identity member of the groups. This is why moving from one configuration to another has an associated energy cost proportional to the distance from a resting state configuration, since under the statistical mechanics formulation, the Boltzmann-Gibbs distribution tells us that physical systems "prefer" to visit low energy states more than high energy states. Thus, the energy is expressed as the summation of the local energy values associated with the multi-state variables which model the entire structure.

### 3.3 Combinatorial Description of the Partition Function

In order to calculate the partition function it is convenient to formulate the problem from an analytic combinatorics point of view [6]. The first step is to define  $N$  as the combinatorial class describing the energy values of the entire structure. Thus, the counts  $N(n)$  (see appendix A for definitions and notations used hereafter) describing the number of configurations  $C$  having exactly energy equal to  $n$ , i.e., the counting sequence of the combinatorial class  $N$ . Furthermore, according to this combinatorial formulation, the partition function  $Z$  is just the ordinary generating function of the combinatorial class  $N$  evaluated in  $z = e^{-\beta}$  (see equation (9)). In addition, to calculate the counts  $N(n)$ , the self-similarity structure of the algebraic structures presented in figure 3 resulting from the statistical mechanics modelization can be exploited by decomposing the calculation by levels. Specifically, a combinatorial class can be assigned to each of the levels comprising the structure to describe its

energy values. In turn, as any particular value of the energy of the structure is the result of the summation of the local energy values of the multi-state variables of the entire structure. Assuming structures with  $k$  levels, being  $k$  a structural parameter that accounts for the number of groups involved in the iterated wreath product operation, the combinatorial class  $N$  can be expressed using the language of admissible combinatorial structures in terms of the combinatorial classes  $N_i$  (see figure 3) where each class  $N_i$  belongs to level  $i$  with  $1 \leq i \leq k$  as follows:

$$N = \overbrace{N_1 \times N_2 \times N_3 \times \cdots \times N_k}^{k \text{ times}} \tag{6}$$

According to the previous combinatorial specification, it is easy to deduce that the counts  $N(n)$  can be expressed by the convolution:

$$N(n) = \sum_{n_1=0}^n \sum_{n_2=0}^{n-n_1} \cdots \sum_{n_k=0}^{n-n_1-n_2-\cdots-n_{k-1}} N_1(n_1)N_2(n_2) \cdots N_k(n_k) \tag{7}$$

Therefore, the generating function of the counts  $N(n)$  is expressed as the product of the generating functions of the combinatorial classes describing the values of energy associated with each of the levels comprising the structure:

$$N(z) = \prod_{i=1}^k N_i(z) \tag{8}$$

Thus, one finally gets for the partition function the general expression:

$$Z = \sum_{n \geq 0} N(n)e^{-\beta n} = N(z)|_{z=e^{-\beta}} = \prod_{i=1}^k N_i(e^{-\beta}) \tag{9}$$

Moreover, it is important to note that the combinatorial description of each of the classes  $N_i$  is identical. The structural differences between each level are in terms of the number of multi-state variables and the number of states in which such variables can be found. Let us suppose a level  $i$  containing just  $j$  multi-state variables of  $m$  states. The possible local values of the energy are obtained as the summation of the local energy values associated to each of the multi-state variables comprising the level. Therefore, the combinatorial structure of the energy values is that of integer compositions (see Appendix A) but with certain particularities.

Specifically, the combinatorial description is that of an integer composition whose parts are only allowed to be taken from the set  $\{1, 2, 3, \dots, m\}$  and with the number of parts fixed by the number of multi-state variables (i.e.,  $j$  variables in this example), being the size of the composition equal to the energy

values. To express this fact in terms of the symbolic language of analytic combinatorics [6], the first step is to define the combinatorial class associated to the integers  $I$ . Let the size of each integer its value, then the counting sequence  $I_n$  associated to the class  $I$  is  $I_n = 1$  for  $n \geq 1$  corresponding to the fact that there is exactly one object in  $I$  for each size  $n \geq 1$ . If integers are represented by small balls, one has  $I = \{1, 2, 3, \dots\} = \{\bullet, \bullet\bullet, \bullet\bullet\bullet, \dots\} = SEQ_{\geq 1}\{\bullet\}$ . The combinatorial specification of the class of compositions made of  $j$  summands,  $j$  a fixed integer can be expressed as  $SEQ_j(I) = SEQ_j(SEQ_{\geq 1}\{\bullet\})$ . Denoting as  $I^{\{1, \dots, m\}}$  the combinatorial class associated to the subset of the integers  $\{1, 2, 3, \dots, m\}$ , one finally has that the combinatorial description of the class of integer compositions  $N_i$  (for a generic level  $i$  of the structure) made of  $j$  summands, whose parts are only allowed to be taken from the set  $\{1, 2, 3, \dots, m\}$ , simply write:

$$N_i = SEQ_j(I^{\{1, \dots, m\}}) = \overbrace{I^{\{1, \dots, m\}} \times I^{\{1, \dots, m\}} \times I^{\{1, \dots, m\}} \times \dots \times I^{\{1, \dots, m\}}}^{j \text{ times}} \quad (10)$$

The result obtained in expression (10) permit us to express the generating function associated with the energy counts  $N_i$  corresponding to a level containing just  $j$  multi-state variables of  $m$  states:

$$N_i(z) = [I^{\{1, \dots, m\}}(z)]^j \quad (11)$$

However, it is important to remind that the previous expression must be further developed to take into account the particular energy model used. The specific mapping between the configurations of the elements from the sets  $\Omega_m$  (as a result of the group actions) and the energy states is yet to be defined. In the following sections, expression (11) is particularized for the energy models resulting when considering the symmetries imposed by permutation groups.

## 4 Group Actions under the Permutation Group $P_m$

### 4.1 The Energy Model

To understand the energy model used when the action groups involved in the wreath product operation are permutation groups, figure 4 provides an example of the structure of algebraic connectivity of a 3-fold iterated wreath-product operation and its entire modelization from a statistical physics perspective. The iterated wreath product operation is  $(P_4 \wr P_3) \wr P_2$ , and the groups involved are permutation groups. Specifically,  $P_k$  denotes the permutation group of order  $k!$ , i.e.,  $|P_k| = k!$ , where  $k \in \{2, 3, 4\}$ . The graph on the left side of the figure

shows the hierarchical structure revealing the algebraic connectivity between groups that result when unfolding the 3-fold wreath product operation. Similarly, the mapping of such structure into a hierarchy of multi-state variables is also shown at the bottom of this structure. The branching factors associated to each level of the structure are in direct correspondence with the number of elements of the sets  $\Omega_2 = \{c_1, c_2\}$ ,  $\Omega_3 = \{c_1, c_2, c_3\}$  and  $\Omega_4 = \{c_1, c_2, c_3, c_4\}$  where each of the permutation groups  $P_2$ ,  $P_3$  and  $P_4$  are respectively acting.

The right side of the graph illustrate the assignments of permutation configurations to local energy values for the permutation groups  $P_2$  and  $P_3$  respectively according to the energy model used. More specifically, the mechanism of assignment of configurations of the elements of the sets  $\Omega_2$  and  $\Omega_3$  (where the groups  $P_2$  and  $P_3$  are respectively acting) to multi-state variable states (i.e. local energy values) is based on the aforementioned idea that moving the system away from its resting state has an associated cost. The table shows the mapping between group elements configurations and energy states for the aforementioned permutation groups. The resting state configuration is always represented by the identity member of the permutation group (the fixed point permutation) or in other words, the sub-index associated with any of the group elements is in concordance with their relative position (e.g.  $c_1c_2c_3$ ). The cost is defined in terms of the distance of configurations (i.e., permutation group elements) with respect to the resting state configuration represented by the identity member of the permutation groups. Specifically, the distance function accounts for the number of discrepancies of elements positions with respect to the fixed point permutation (e.g.  $c_1c_2c_3$  for the set  $\Omega_3$  or  $c_1c_2$  for the set  $\Omega_2$ ). For instance, for the configuration  $c_1c_3c_2$  there are two discrepancies (element  $c_3$  is in position 2 and element  $c_2$  in position 3). Similarly, there are also two discrepancies for the configuration  $c_2c_1c_3$ , while there are three for  $c_3c_1c_2$ . In addition, it is important to note that the multi-state variable states are degenerate, because the number of elements of the groups (i.e., the number of configurations) is bigger than the cardinality of its set of states.

In the following, for ease of exposition, it is assumed that the ( $k$ -folded) iterated wreath product operations studied follow the scheme:  $(\dots(((P_m^k \wr P_m^{k-1}) \wr P_m^{k-2}) \wr \dots) \wr P_m^2) \wr P_m^1)$ , where  $P_m^k = P_m^{k-1} = P_m^{k-2} = \dots = P_m^2 = P_m^1 = P_m$ . In other words, all the nodes comprising the entire hierarchical structure of  $k$  levels are representing the permutation group of  $m!$  elements  $P_m$ , being  $m$  any positive integer value.

## 4.2 Mapping Between Configurations and Energy States

According to the energy model explained in section 4.1, the size of the permutation group is directly related to the number of configurations of the elements of the group, whereas the number of elements of the sets (i.e.,  $m$  in the example

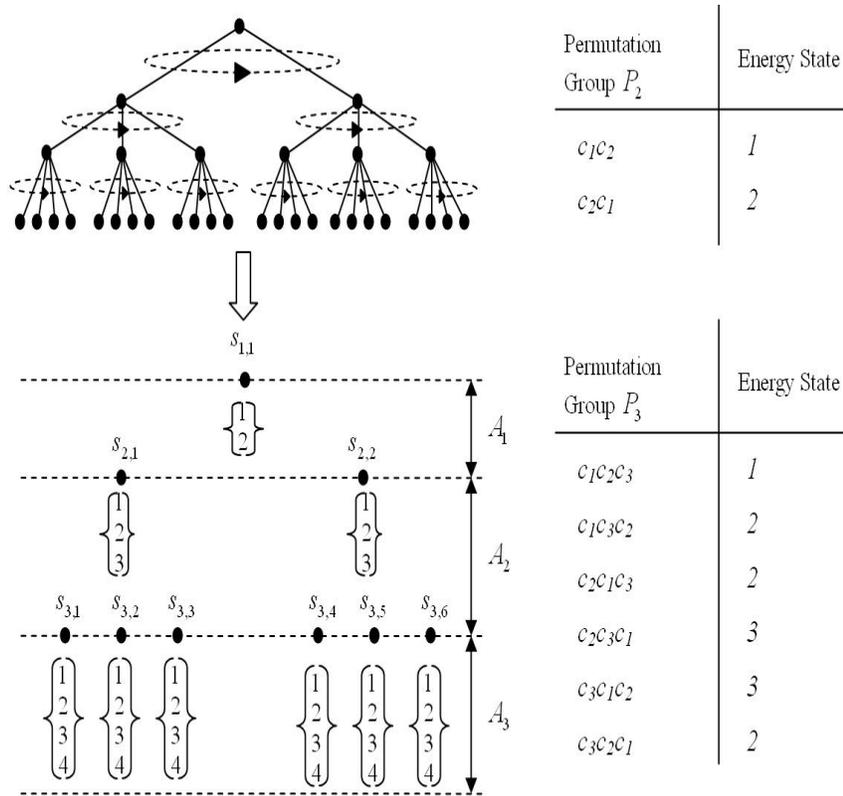


Figure 4: Graphic illustration of the structure of algebraic connectivity of a 3-fold iterated wreath-product operation and its modelization from a statistical physics perspective. The iterated wreath product operation is  $(P_4 \wr P_3) \wr P_2$ , and the groups involved are permutation groups. Specifically,  $P_k$  denotes the symmetric group of order  $k!$ , i.e.,  $|P_k| = k!$ . The graph on the left side shows the hierarchical structure revealing the algebraic connectivity between groups that result when unfolding the 3-fold wreath product operation. Similarly, the mapping of such structure into a hierarchy of multi-state variables is also shown at the bottom of this structure. The branching factor associated to each level of the structure are in direct correspondence with the number of elements of the sets  $\Omega_2 = \{c_1, c_2\}$ ,  $\Omega_3 = \{c_1, c_2, c_3\}$  and  $\Omega_4 = \{c_1, c_2, c_3, c_4\}$  where each of the permutation groups  $P_2$ ,  $P_3$  and  $P_4$  are respectively acting. The right side of the graph illustrate the assignments of permutation configurations to local energy values for the permutation groups  $P_2$  and  $P_3$  respectively according to the energy model used. The variables  $A_i$ , where  $1 \leq i \leq k$  are employed to denote the combinatorial classes used to describe the energy values associated to each level of the structure.

under study) where the permutation groups are acting is related to the cardinality of the local energy values of the multi-state variables. Let us denote by  $A_m^l$  the coefficient describing the mapping between the number of group elements having an energy value equal to  $l$  where  $1 \leq l \leq m$ , for the permutation group  $P_m$ . From an Analytic Combinatorics point of view this coefficients can be interpreted as the counting sequence of a combinatorial class. Let us denote this combinatorial class as  $A^{(m)}$ . It can be shown (see appendix B for details) that the counting sequence  $A_m^l$  expressing the mappings follows the expression:

$$A_m^l = \begin{cases} 1 & l = 1 \\ \binom{m}{l} A_l^l & 1 < l \leq m \end{cases} \tag{12}$$

Where the coefficients  $A_l^l$  are given by:

$$A_l^l = \sum_{j=2}^l (-1)^j \frac{l!}{j!} \tag{13}$$

Thus, the generating function  $A^{(m)}(z)$  corresponding to the combinatorial class  $A^{(m)}$  can be expressed as:

$$A^{(m)}(z) = z + \sum_{l=2}^m A_m^l z^l = z + \sum_{l=2}^m \binom{m}{l} A_l^l z^l \tag{14}$$

The existence of degenerated states means that the counting sequence associated to the combinatorial class describing the local energy values (i.e.,  $I^{\{1, \dots, m\}}$ ) of the multi-states variables has changed because of the existence of multiple objects (for any given size), instead of the one-to-one mapping between size and number of combinatorial objects that existed before. More specifically, a state with energy equal to  $l$  (where  $1 \leq l \leq m$ ) has now associated  $A_m^l$  configurations. Thus, the existence of degenerated states leads simply to the substitution of the combinatorial class  $N_i$  by the combinatorial class  $A_i$ , where  $1 \leq i \leq k$  (see the variables attached to each level of the hierarchy of multi-state variables in figure 4) that describes the energy values associated to each level of the structure. Specifically, the combinatorial class  $I^{\{1, \dots, m\}}$  is substituted by the class  $A^{(m)}$ . Re-writing expression (10) finally produces:

$$A_i = SEQ_j(A^{(m)}) = \overbrace{A^{(m)} \times A^{(m)} \times A^{(m)} \times \dots \times A^{(m)}}^{j \text{ times}} \tag{15}$$

### 4.3 Derivation of the Partition Function

Taking into account the formulation presented in the previous sections, the combinatorial specification of the class  $N$  when considering global permutation symmetries can be finally written:

$$\begin{aligned}
N = & A^{(m)} \times \overbrace{(A^{(m)} \times A^{(m)} \times \dots \times A^{(m)})}^{m \text{ times}} \times \overbrace{(A^{(m)} \times A^{(m)} \times \dots \times A^{(m)})}^{m^2 \text{ times}} \times \dots \\
& \dots \times \overbrace{(A^{(m)} \times A^{(m)} \times \dots \times A^{(m)})}^{m^{k-1} \text{ times}} \quad (16)
\end{aligned}$$

Thus, the generating function associated to the counts  $N(n)$  corresponding to the symmetries imposed by the permutation group can be finally expressed as:

$$N(z) = [A^{(m)}(z)]^\lambda \quad (17)$$

Where the parameter  $\lambda$  is defined as:

$$\lambda = \frac{1 - m^k}{1 - m} \quad (18)$$

It is important to note that the ground state of the structure has an associated energy value  $n_{min}$  that is equal to the parameter  $\lambda$  defined above. Similarly, the maximum energy value  $n_{max}$  is equal to  $m\lambda$ . Using the generating function  $N(z)$  obtained in (17), a closed expression for the partition function  $Z$  can be obtained:

$$Z = N(z)|_{z=e^{-\beta}} = e^{-\beta\lambda} \left( 1 + \sum_{l \geq 2}^m \binom{m}{l} e^{-\beta(l-1)} A_l^l \right)^\lambda \quad (19)$$

Moreover, after doing some algebra (the complete derivation is provided in appendix B) it can also be shown that the counts  $N(n)$  can be expressed in a closed form in terms of partial exponential Bell polynomials [4]:

$$N(n) = \frac{\lambda!}{n!} B_n^k(x_1, x_2, \dots, x_{n-\lambda+1}) \quad (20)$$

where the following expression holds for the polynomial variables  $x_l$ :

$$x_l = \begin{cases} l! A_m^l & l \leq m \\ 0 & l > m \end{cases} \quad (21)$$

#### 4.4 Asymptotic Expansion

The expression (19) corresponding to the partition function is complicated by the presence of a summation involving combinatorial factors. In order to obtain a more compact and at the same time, a more tractable expression for the partition function, this section is devoted to the calculation of an asymptotic expansion of the partition function. To this end, the theory of singularity

analysis is used. This theory is dedicated to the process of extracting asymptotic information from counting generating functions. The basic principle of singularity analysis is the existence of a general correspondence between the asymptotic expansion of a function near its dominant singularities and the asymptotic expansion of the function's coefficients. Specifically, the method is mainly based on Cauchy's coefficient formula used in conjunction with special contours of integration known as Hankel contours. Let us denote as  $g_m$  and  $h_m$  the following sequences:

$$g_m = e^\beta \sum_{l \geq 0} \binom{m}{l} e^{-\beta l} d_l \tag{22}$$

$$h_m = 1 + e^\beta \sum_{l \geq 2} \binom{m}{l} e^{-\beta l} A_l^l \tag{23}$$

The coefficients  $d_l$  in expression (22) correspond to the subfactorial function [18, 6]. Taking into account that  $d_0 = 1$  and  $d_1 = 0$ , the sequences  $g_m$  and  $h_m$  are related through the expression:

$$h_m = 1 - e^\beta + g_m \tag{24}$$

The first step to apply singularity analysis is to calculate the generating function of  $g_m$ . Furthermore, this sequence can be interpreted as the result of the binomial convolution of two sequences (see definition A.8 in appendix A). Namely, the sequence  $g_m^1 = e^{-\beta m} A_m^m$  and the sequence  $g_m^2 = 1$ . Thus, the generating function  $G(z)$  associated to the sequence  $g_m$  can be expressed as the product of the generating functions  $G_1(z)$  and  $G_2(z)$  corresponding to the counting sequences  $g_m^1$  and  $g_m^2$  respectively:

$$g_m = e^\beta g_m^1 \oplus g_m^2 \quad \Rightarrow \quad \frac{g_m}{m!} = e^\beta \sum_{l \geq 0} \frac{g_m^1}{l!} \frac{g_{m-l}^2}{(m-l)!} \tag{25}$$

After doing some algebra the exponential generating functions associated to the sequences  $g_m^1$  and  $g_m^2$  read respectively:

$$G_1(z) = \sum_{m \geq 0} g_m^1 \frac{z^m}{m!} = \frac{e^{e^{-\beta} z}}{1 - e^{-\beta} z} \tag{26}$$

$$G_2(z) = \sum_{m \geq 0} g_m^2 \frac{z^m}{m!} = e^z \tag{27}$$

Hence, the exponential generating function of the sequence  $g_m$  finally reads:

$$G(z) = e^\beta G_1(z) G_2(z) = e^\beta \frac{e^{z(1-e^{-\beta})}}{1 - e^{-\beta} z} \tag{28}$$

In order to obtain an asymptotic expansion for the sequence  $h_m$ , the first step is to apply the method of singularity analysis to the generating function  $G(z)$ . Thus, the first step consist in expressing the coefficients  $g_m$  of the generating function  $G(z)$  as a contour integral using the Cauchy coefficient formula:

$$\frac{g_m}{m!} = [z^m]G(z) = \frac{1}{2\pi i} \oint_C G(z) \frac{dz}{z^{m+1}} = \frac{1}{2\pi i} \oint_C e^\beta \frac{e^{z(1-e^{-\beta})}}{1-e^{-\beta}z} \frac{dz}{z^{m+1}} \quad (29)$$

Using the change of variables  $e^{-\beta}z = u$  in the above integral and re-arranging the resulting expression one gets:

$$\frac{g_m}{m!} = [z^m]G(z) = \frac{e^{-\beta(m-1)}}{2\pi i} \oint_C \frac{e^{-u}}{1-u} e^{ue^\beta} \frac{du}{u^{m+1}} \quad (30)$$

The second step is to express the contour integral using a Hankel contour. To this end, under the change of variables  $u = 1 + \frac{t}{m}$ , the kernel  $u^{-m-1}$  in the integral (30) transform asymptotically into an exponential. Using the aforementioned change of variables in the previous expression together with a Hankel contour one gets:

$$\begin{aligned} \frac{g_m}{m!} &= \frac{e^{-\beta(m-1)}}{2\pi i} \oint_{+\infty}^{(0)} \frac{e^{-(1+\frac{t}{m})}}{(-t)} m e^{e^\beta(1+\frac{t}{m})} e^{-t} \frac{dt}{m} = \\ &= \frac{e^{-\beta(m-1)}}{2\pi i} \oint_{+\infty}^{(0)} (-t)^{-1} e^{-t} \left\{ 1 - \frac{t}{m}(1-e^\beta) + \frac{t^2}{m^2}(1-e^\beta)^2 + \dots \right\} \cong \\ &\cong e^{-\beta(m-1)} e^{-(1-e^\beta)} \Gamma(1) \end{aligned} \quad (31)$$

Denoting as  $\xi = e^{-\beta}$  one finally gets the following asymptotic approximation for the coefficients  $h_m$

$$h_m \cong 1 - \frac{1}{\xi} + m! \xi^{m-1} e^{-(1-\frac{1}{\xi})} \quad (32)$$

## 5 Group Actions under the Cyclic Subgroup $C_m \subset P_m$

### 5.1 The Energy Model

Following a similar scheme to that employed in section 4.1, figure 5 provides another example of a 3-fold wreath-product operation and its statistical physics modelization. The energy model is now particularized for the case in which the action groups involved in the wreath product operation are cyclic groups. It is important to emphasize that the actions of the permutation group  $P_m$

and its subgroups acting on a set of  $m$  elements consists on permuting its elements. Thus, the iterated wreath product operation is now  $(C_4 \wr C_3) \wr C_2$ , and the groups involved are cyclic groups. Specifically, without a loss of generality let us suppose that  $C_k \subset P_k$  denotes a transitive cyclic subgroup of order  $k$ , i.e.,  $|C_k| = k$  belonging to the permutation group  $P_k$ . For instance, using the standard cyclic notation used for expressing permutations [6], the elements of the groups  $C_3 \subset P_3$  and  $C_4 \subset P_4$  that compose the wreath-product operation of the figure are respectively,  $C_3 = \{e, (123), (321)\}$  and  $C_4 = \{e, (1234), (13)(24), (1432)\}$ , corresponding to the tables that are shown at the right side of the figure. In these tables, each element of these groups is represented as a permutation of the elements from the sets  $\Omega_3$  and  $\Omega_4$ , respectively. The table also shows the mapping between group elements configurations and local energy states for the aforementioned permutation groups. The resting state configuration is always represented by the identity member of the permutation group (the fixed point permutation) or in other words, the sub-index associated with any of the group elements is in concordance with their relative position (e.g.  $c_1c_2c_3$ ). As before, the fixed point permutation is always assigned an energy value equal to 1.

Moreover, the graph on the left side of the figure shows the hierarchical structure revealing the algebraic connectivity that result when unfolding the 3-fold wreath product operation. Similarly, the mapping of such structure into a hierarchy of multi-state variables is also shown at the bottom of the figure (left side). The branching factors associated to each level of the structure are in direct correspondence with the number of elements of the sets  $\Omega_2 = \{c_1, c_2\}$ ,  $\Omega_3 = \{c_1, c_2, c_3\}$  and  $\Omega_4 = \{c_1, c_2, c_3, c_4\}$  where each of the cyclic groups  $C_2$ ,  $C_3$  and  $C_4$  are respectively acting. The right side of the graph illustrate the assignments of cyclic permutation configurations to local energy values for the cyclic subgroups  $C_2$  and  $C_4$  according to the energy model used. The mechanism of assignment of configurations of the elements of the sets  $\Omega_2$  and  $\Omega_3$  to multi-state variable states (i.e. local energy values) is based on the aforementioned idea that moving the system away from the resting state (represented by the identity member of those groups) has an associated cost. However, the cost is now defined in terms of the number of circular shifts with respect to the fixed point permutation, i.e., the identity member of the cyclic subgroup. For instance, the configuration  $c_2c_3c_1$  is the result of one position left circular shift from the resting state configuration  $c_1c_2c_3$ . Similarly, the configuration  $c_3c_1c_2$  is the result of one position right circular shift, or the configuration  $c_3c_4c_1c_2$  is two circular shifts (both left or right) away from the fixed point permutation  $c_1c_2c_3c_4$ . Furthermore, it is important to note that for this scheme, the number of states that can be associated to the multi-state variables is not equal to the branching factor  $m$  (i.e., the permutation size). Furthermore, according to this energy model the multi-state variable states are

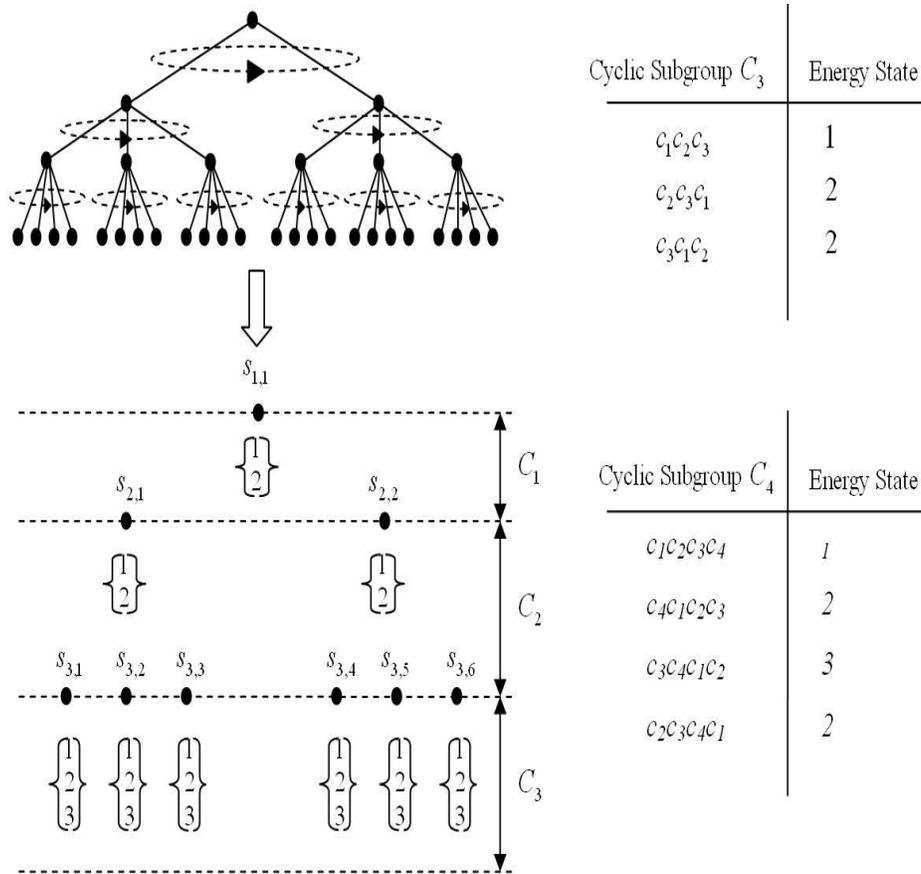


Figure 5: Another example of the structure of algebraic connectivity of a 3-fold wreath-product operation and its modelization from a statistical physics perspective. In this case the groups involved in the wreath product operation  $(C_4 \wr C_3) \wr C_2$  are the transitive cyclic subgroups  $C_4 \subset S_4$ ,  $C_3 \subset S_3$  and  $C_2 \subset S_2$ , where  $C_k$  denotes the cyclic group of order  $k$ , i.e.,  $|C_k| = k$ . The graph on the left side shows the resulting hierarchical structure when unfolding the wreath product and the mapping of such structure into a hierarchy of multi-state variables. The values of the branching factor associated to each level of the structure is in direct correspondence with the number of elements of the sets  $\Omega_2 = \{c_1, c_2\}$ ,  $\Omega_3 = \{c_1, c_2, c_3\}$  and  $\Omega_4 = \{c_1, c_2, c_3, c_4\}$  where each of the cyclic subgroups  $C_2$ ,  $C_3$  and  $C_4$  are respectively acting. The right side of the graph illustrate the assignments of cyclic permutation configurations to local energy values for the cyclic subgroups  $C_2$  and  $C_4$  according to the energy model used. Similarly, the variables  $C_i$ , where  $1 \leq i \leq k$  are employed to denote the combinatorial classes used to describe the energy values associated to each level of the structure.

again degenerate, as the number of configurations is bigger than the cardinality of its set of states.

In the next section, following a similar schema to that used in section 4, it is assumed that the iterated wreath product operations studied are of the form:  $(\dots(((C_m^k \wr C_m^{k-1}) \wr C_m^{k-2}) \wr \dots) \wr C_m^2) \wr C_m^1$ , where  $C_m^k = C_m^{k-1} = C_m^{k-2} = \dots = C_m^2 = C_m^1 = C_m \subset P_m$ .

### 5.2 Mapping Between Configurations and Energy States

In a similar way to what occurred before (when permutation groups are considered), the existence of a mapping expressing the correspondence between group elements configurations and energy states, as a result of the cyclic group actions, leads to substitute again the combinatorial class  $N_i$  with  $1 \leq i \leq k$  by a new class denoted as  $C_i$  (see the variables attached to each level of the hierarchy of multi-state variables in figure 5). Specifically, the combinatorial class  $I^{\{1, \dots, m\}}$  is substituted by the class  $C^{(m)}$ . Re-writing expression (10) finally produces:

$$C_i = SEQ_j(C^{(m)}) = \overbrace{C^{(m)} \times C^{(m)} \times C^{(m)} \times \dots \times C^{(m)}}^{j \text{ times}} \tag{33}$$

where the class  $C^{(m)}$  is used to express such mappings. Let us denote the counting sequence of the class  $C^{(m)}$  as  $C_m^l$ . These coefficients, i.e.,  $C_m^l$  describe the mapping between the number of elements from the cyclic group having an energy value equal to  $l$  for a subgroup  $C_m \subset P_m$  associated to a permutation of size equal to  $m$ . These mappings follow the expression:

$$C_m^l = \begin{cases} 1 & l = 1 \\ 2 & 1 < l \leq \mu \\ 2^{m \bmod 2} & l = \mu + 1 \end{cases} \tag{34}$$

Where the parameter  $\mu$  is defined as:

$$\mu = \frac{m - m \bmod 2}{2} \tag{35}$$

and the function *mod* stands for the remainder function. It is important to note that the range of local energy values for the multi-state variables belongs now to the integer interval  $[1.. \mu + 1]$ . Thus, the generating function  $C^{(m)}(z)$  corresponding to the combinatorial class  $C^{(m)}$  reads:

$$C^{(m)}(z) = \sum_{l \geq 1}^{\mu+1} C_m^l z^l = z \left( 1 + 2^{m-2\mu} z^\mu + 2z \frac{1 - z^{\mu-1}}{1 - z} \right) \tag{36}$$

### 5.3 Derivation of the Partition Function

Taking into account the formulation presented in section 4, the combinatorial specification of the class  $N$ , when considering cyclic permutation symmetries, is obtained by simply substituting the combinatorial class expressing the mappings between configurations and states as a result of the cyclic group actions:

$$\begin{aligned}
 N = C^{(m)} \times & \overbrace{(C^{(m)} \times C^{(m)} \times \dots \times C^{(m)})}^{m \text{ times}} \times \overbrace{(C^{(m)} \times C^{(m)} \times \dots \times C^{(m)})}^{m^2 \text{ times}} \times \dots \\
 & \dots \times \overbrace{(C^{(m)} \times C^{(m)} \times \dots \times C^{(m)})}^{m^{k-1} \text{ times}}
 \end{aligned} \tag{37}$$

Thus, the generating function associated to the counts  $N(n)$  for cyclic permutation symmetries can be finally expressed as:

$$N(z) = [C^{(m)}(z)]^\lambda \tag{38}$$

It is important to note that in this case the ground state of the hierarchy of multi-state variables associated to the structures under study, i.e.,  $n_{min}$  is also equal to the parameter  $\lambda$ . However, the maximum value that can be attained by the energy function is now  $n_{max} = (\mu + 1)\lambda$ , which differs from that found when considering the actions induced by the permutation group. Using expression (9) together with the expression of the generating function  $C^{(m)}(z)$ , after doing some algebra the partition function finally reads:

$$Z = e^{-\beta\lambda} \left( 1 + 2^{m-2\mu} e^{-\beta\mu} + 2e^{-\frac{\beta\mu}{2}} \frac{\sinh(\frac{\beta(\mu-1)}{2})}{\sinh(\frac{\beta}{2})} \right)^\lambda \tag{39}$$

Similarly, the counts  $N(n)$  can also be expressed in a closed form in terms of partial exponential Bell polynomials:

$$N(n) = [z^n]N(z) = [z^n][C^{(m)}(z)]^\lambda = \frac{\lambda!}{n!} B_n^k(y_1, y_2, \dots, y_{n-\lambda+1}) \tag{40}$$

where the following expression holds for the polynomial variables  $y_l$ :

$$y_l = \begin{cases} l!C_m^l & l \leq \mu + 1 \\ 0 & l > \mu + 1 \end{cases} \tag{41}$$

## 6 Conclusions

In this paper iterated wreath product groups were introduced as powerful group theoretic constructions to characterize complex symmetries. More specifically, by iterating the basic scheme of a wreath-product operation,  $k$ -folded

wreath product groups were defined. The importance of these algebraic structures was put forward as a way to describe the generation of complex symmetries in a broad range of research disciplines. Afterwards, the resulting hierarchical structures obtained when considering the actions induced by permutation groups were studied from a statistical physics perspective to illustrate the potential of the mathematical techniques of analytic combinatorics. The resulting algebraic structures were modeled as Cayley trees, whereas the interactions between the nodes comprising the structures were based on the actions imposed by those groups. Furthermore, the partition functions induced by these algebraic constructions were expressed as generating function of energies to permit their treatment from the point of view of analytic combinatorics. The advantages of the symbolic and the complex asymptotic methods of the theory were emphasized as a way to describe complex combinatorial interactions that permit to set up functional relations between partition functions, and also as a way of extracting asymptotic information useful when calculating approximations or deriving more tractable expressions. The most important result of this paper is the fact that closed expressions for the partition functions analyzed were obtained, illustrating the potential of these mathematical techniques.

## Appendix A. Definitions and Notations

The goal of this appendix is to provide the definitions of the mathematical concepts and notations used throughout this paper (see [6] for an extensive review) together with the derivations of the most important mathematical expressions.

**Definition A.1** (Combinatorial class). A combinatorial class is a finite or denumerable set in which a size function is defined, satisfying the following conditions: (1) the size of an element is a non-negative integer. (2) The number of elements of any given size is finite. If  $A$  is a class, the size of an element  $\alpha \in A$  is denoted as  $|\alpha|$ .

**Definition A.2** (Counting sequence). The counting sequence of a combinatorial class  $A$  is the sequence of integers  $(A_n)_{n \geq 0}$  where  $A_n$  is the number of objects in class  $A$  that have size  $n$ .

**Definition A.3** (Generating function). The generating function of a sequence  $A_n$  is the formal power series, where  $w_n = 1$  for the ordinary case and  $w_n = n!$  for the exponential case.

$$A(u) = \sum_{n \geq 0} A_n \frac{u^n}{w_n} = \sum_{\alpha \in A} \frac{u^{|\alpha|}}{w_n} \quad (42)$$

**Definition A.4** (Bivariate generating function). The bivariate generating function (BGF) either ordinary or exponential of an array  $f_{n,k}$  are the formal power series in two variables defined by:

$$f(z, u) = \begin{cases} \sum_{n \geq 0} \sum_{k \geq 0} f_{n,k} z^n u^k & \text{(ordinary BGF)} \\ \sum_{n \geq 0} \sum_{k \geq 0} f_{n,k} u^k \frac{z^n}{n!} & \text{(exponential BGF)} \end{cases} \quad (43)$$

**Definition A.5** (Coefficient extraction). We generally let  $A_n = w_n[u^n]A(u)$  denote the operation of extracting the coefficient of  $u^n$  in the formal power series (A.3).

$$A_n = w_n[u^n] \left( \sum_{n \geq 0} A_n \frac{u^n}{w_n} \right) = \frac{1}{2\pi i} \oint_C w_n A(u) \frac{du}{u^{n+1}} \quad (44)$$

**Definition A.6** (Integer composition). A composition of an integer  $n$  is a sequence  $(x_1, x_2, x_3, \dots, x_k)$  of integers (for some  $k$ ) such that:

$$n = x_1 + x_2 + \dots + x_k \quad \text{and} \quad x_j \geq 1, \quad 1 \leq j \leq k \quad (45)$$

The  $x_i$  are called the summands or the parts and the quantity  $n$  is called the size.

**Definition A.7** (Integer partition). A partition of an integer  $n$  is a sequence  $(x_1, x_2, x_3, \dots, x_k)$  of integers (for some  $k$ ) such that:

$$n = x_1 + x_2 + \dots + x_k \quad \text{and} \quad x_1 \geq x_2 \geq \dots \geq x_k \quad (46)$$

The  $x_i$  are called the summands or the parts and the quantity  $n$  is called the size.

**Definition A.8** (Binomial Convolution). Let  $a(u)$ ,  $b(u)$  and  $c(u)$  be exponential generating functions, with  $a(u) = \sum_{n \geq 0} a_n \frac{u^n}{n!}$ , and so on. The binomial convolution formula is:

$$\text{if } a(u) = b(u)c(u), \quad \text{then } a_n = \sum_{k=0}^n \binom{n}{k} b_k c_{n-k} = b_n \oplus c_n \quad (47)$$

where  $\binom{n}{k} = n!/(k!(n-k)!)$  represents a binomial coefficient.

**Definition A.9** (Cartesian Product of Combinatorial classes). The cartesian product construction applied to two combinatorial classes  $B$  and  $C$  forms ordered pairs,  $A = B \times C \Leftrightarrow A = \{\alpha = (\beta, \gamma) | \beta \in B, \gamma \in C\}$ , with the size of a pair  $\alpha = (\beta, \gamma)$  being defined by  $|\alpha|_A = |\beta|_B + |\gamma|_C$ . By considering all possibilities, the counting sequences corresponding to  $A, B, C$  are related by the convolution relation:

$$A_n = \sum_{k=0}^n B_k C_{n-k} \tag{48}$$

Furthermore, the convolution relation is the formula for a product of two power series:  $A(u) = B(u)C(u)$ .

**Definition A.10** (Admissible Combinatorial Constructions). Let  $\Phi$  be an  $m$ -ary construction that associates to any collection of classes  $B^1, B^2, \dots, B^m$  a new class  $A = \Phi[B^1, B^2, \dots, B^m]$ . The construction  $\Phi$  is admissible if and only if the counting sequence  $A_n$  of  $A$  only depends on the counting sequences  $B_n^1, B_n^2, \dots, B_n^m$  of  $B^1, B^2, \dots, B^m$ . For such an admissible construction, there then exists a well-defined operator  $\Psi$  acting on the corresponding ordinary generating functions  $A(u) = \Psi[B^1(u), B^2(u), \dots, B^m(u)]$ .

- **Cartesian product:** This construction  $A = B \times C$  forms all possible ordered pairs in accordance with definition A.9. The size of a pair is obtained additively from the size of components.
- **Sequence construction:** If  $B$  is a combinatorial class then the sequence class  $A = SEQ(B)$  is defined as the infinite sum:

$$A = SEQ(B) = \{\epsilon\} + B + (B \times B) + (B \times B \times B) + \dots \tag{49}$$

The construction  $A = SEQ(B)$  defines a proper class satisfying the finiteness condition for sizes if and only if  $B$  contains no object of size 0, with  $\epsilon$  being a neutral structure (of size 0) which plays a similar role to that of the "empty" word in formal language theory. In other words, we have  $A = \{(\beta_1, \beta_2, \dots, \beta_l) | l \geq 0, \beta_j \in B\}$ , where the neutral structure corresponds to  $l = 0$ . It follows that the size of an object  $\alpha \in A$  is to be taken as the sum of the sizes of its components:  $\alpha = (\beta_1, \beta_2, \dots, \beta_l) \Rightarrow |\alpha| = |\beta_1| + \dots + |\beta_l|$ . Therefore, the ordinary generating function associated to the sequence construction is as follows:

$$A = SEQ(B) \Rightarrow A(u) = 1 + B(u) + B^2(u) + \cdots = \frac{1}{1 - B(u)} \quad (50)$$

Similarly, sequences whose number of components are exactly  $k$ , larger or equal than  $k$  are expressed as  $SEQ_k$  and  $SEQ_{\geq k}$  respectively, admitting the translation into ordinary generating functions:

$$A = SEQ_k(B) = \overbrace{B \times B \times \cdots \times B}^{k \text{ times}} \Rightarrow A(u) = B(u)^k \quad (51)$$

$$A = SEQ_{\geq k}(B) = \sum_{j \geq k} B^j \cong B^k \times SEQ(B) \Rightarrow A(u) = \frac{B(u)^k}{1 - B(u)} \quad (52)$$

## Appendix B. Derivation of the Most Important Equations

**Equations (12) and (13)** (Coefficients expressing the mappings between the elements of the permutation group and local energy values). The coefficients  $A_m^l$  describe the mapping between the number of configurations having an energy value equal to  $l$ , where  $1 \leq l \leq m$ . Taking into account that the size of the permutation is described by the parameter  $m$ , it is easy to verify the following equality for these coefficients:

$$\sum_{l=1}^m A_m^l = 1 + \sum_{l=2}^m A_m^l = m! \quad (53)$$

In turn, the above equality can be associated to a binomial convolution (see definition A.8) of two integer sequences  $b_m$  and  $c_m$  aimed at decorrelating the functional dependence of the bivariate coefficients  $A_m^l$  as it follows:

$$a_m = m! = \sum_{l=1}^m A_m^l = b_m \oplus c_m = \sum_{l=1}^m \binom{m}{l} b_l c_{m-l} \quad (54)$$

The binomial convolution holds when  $b_m = A_m^m$  and  $c_m = 1$  and equation (53) finally reads:

$$\sum_{l=1}^m A_m^l = 1 + \sum_{l=2}^m \binom{m}{l} A_l^l = m! \quad (55)$$

Thus, providing a system of equations that can be used to obtain the exact values of the coefficients  $A_m^m$ . In particular the following sequence is obtained:  $A_1^1 = 1, A_2^2 = 1, A_3^3 = 2, A_4^4 = 9, A_5^5 = 44, A_6^6 = 265, A_7^7 = 1854, A_8^8 = 14833, A_9^9 = 133496, A_{10}^{10} = 1334961, \dots$  that corresponds to the subfactorial function (i.e., derangements) [18, 6]:

$$A_l^l = \sum_{j=2}^l (-1)^j \frac{l!}{j!} \tag{56}$$

**Equation (20)** (The Counting Sequence of the Generating Function of Energies). Let us start first studying the following bivariate generating function:

$$\Phi(z, u) = \exp(zX(u)) \tag{57}$$

Where  $X(u)$  correspond to the exponential generating function of a combinatorial class  $X$ :

$$X(u) = \sum_{l \geq 0} x_l \frac{u^l}{l!} \tag{58}$$

In addition, the multinomial expansion theorem provides the classic formula:

$$\left(\sum_{k=1}^p x_k\right)^n = \sum_{k_1+k_2+\dots+k_p=n} \frac{n!}{k_1!k_2!\dots k_p!} x_1^{k_1} x_2^{k_2} \dots x_p^{k_p} \tag{59}$$

From the Taylor expansion of the exponential function, the expression (58) together with the multinomial expansion formula (59), the bivariate generating function (57) can be expressed as follows:

$$\begin{aligned} \Phi(z, u) &= \sum_{k \geq 0} \left(\sum_{l \geq 0} x_l \frac{u^l}{l!}\right)^k \frac{z^k}{k!} \\ &= \sum_{k \geq 0} \sum_{k_1+k_2+\dots+k_p=k} \frac{z^{k_1+k_2+k_3+\dots}}{k_1!k_2!k_3!\dots} \left(\frac{x_1}{1!}u\right)^{k_1} \left(\frac{x_2}{2!}u^2\right)^{k_2} \left(\frac{x_3}{3!}u^3\right)^{k_3} \dots \\ &= \sum_{k \geq 0} \sum_{k_1+k_2+\dots+k_p=k} \frac{x_1^{k_1} x_2^{k_2} \dots}{k_1!k_2!\dots (1!)^{k_1} (2!)^{k_2} \dots} z^{k_1+k_2+\dots} u^{k_1+2k_2+\dots} \end{aligned} \tag{60}$$

In order to express (60) in a more compact way, as both summation terms goes to infinite, we can firstly denote the exponential index for the variables  $u$  and  $z$  as follows:

$$\begin{aligned} k_1 + k_2 + k_3 + \dots &= k \\ k_1 + 2k_2 + 3k_3 + \dots &= n \end{aligned} \tag{61}$$

Multiplying and dividing by  $n!$  and using expression (61). The expression (60) can be finally expressed in a more compact form as it is shown below:

$$\begin{aligned} \Phi(z, u) &= \sum_{n \geq 0} \sum_{k \geq 0} \left\{ \sum_{\pi(n,k)} \frac{n!}{k_1!k_2! \dots (1!)^{k_1} (2!)^{k_2} \dots} x_1^{k_1} x_2^{k_2} \dots \right\} \frac{u^n}{n!} z^k \\ &= \sum_{n \geq 0} \sum_{k \geq 0} \sum_{\pi(n,k)} \prod_{j=1}^{n-k+1} \frac{n!}{k_j!(j!)^{k_j}} x_j^{k_j} \frac{u^n}{n!} z^k \end{aligned} \tag{62}$$

More specifically, the coefficients  $\frac{n!}{k_1!k_2! \dots (1!)^{k_1} (2!)^{k_2} \dots}$  can be interpreted as the number of partitions of  $n$  with  $k_1 + 2k_2 + 3k_3 + \dots = n$  where  $k_i$  is the number of parts of size  $i$  and  $k_1 + k_2 + k_3 + \dots = k$  is the number of parts in the partition. Moreover, the summation index  $\pi(n, k)$  stands for the number of partitions of the integer  $n$  into  $k$  summands, where  $n \geq k$ . Thus, the bivariate generating function (57) can be finally expressed in terms of partition polynomials known as the partial exponential Bell polynomials:

$$\Phi(z, u) = \sum_{n \geq 0} \sum_{k \geq 0} B_n^k(x_1, x_2, \dots, x_{n-k+1}) \frac{z^n}{n!} u^k \tag{63}$$

Where each polynomial  $B_n^k(x_1, x_2, \dots, x_{n-k+1})$  contains exactly  $\pi(n, k)$  monomials:

$$B_n^k(x_1, x_2, \dots, x_{n-k+1}) = \sum_{\pi(n,k)} \prod_{j=1}^{n-k+1} \frac{n!}{k_j!(j!)^{k_j}} x_j^{k_j} \tag{64}$$

Taking into account the considerations stated above we can rephrase the exact expression of the coefficients of  $N(u)$  in terms of Bell polynomials as follows:

$$\begin{aligned} N(n) &= [u^n]N(u) \\ &= [u^n](A_m(u))^\lambda \\ &= \frac{\lambda!}{n!} B_n^\lambda(x_1, x_2, \dots, x_{n-\lambda+1}) \end{aligned} \tag{65}$$

In expression (64), as the generating function  $X(u) = A_m(u)$  is the result of an ordinary finite expansion, the polynomials variables  $x_k$  take the form:

$$x_k = \begin{cases} k!A_m^k & k \leq m \\ 0 & k > m \end{cases} \tag{66}$$

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