ENUMERATION OF THE FIRST MULTICYCLIC ISOMORPHISM-FREE LABELLED GRAPHS (EXTENDED ABSTRACT)

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ABSTRACT. Given a fixed connected graph H, a *H-free* graph is one which does not contain a copy of subgraph isomorphic to H. We describe a very general technique which can be applied to enumerate any labelled graphs without copies of H for the first multicyclic components, i.e., connected graphs with n vertices and $(n+k)$ edges for small k. The results are obtained by means of generating functions which are shown to verify a differential equation of heat conduction type, reducing the enumeration of H-free labelled graphs to the enumeration of two types of graphs; graphs with one and only one occurrence of H and graphs with many occurrences of H but necessarily juxtaposed. Then, general methods are presented and used to enumerate the first low-order cyclic components of these two types of graphs. These techniques are less efficient and impracticable for greater k, but give the first combinatorial results for labelled connected H-free graphs. Furthermore, the methods are illustrated by the examples of the enumeration of C_3-free or triangle-free and K_4-free labelled graphs.

RÉSUMÉ. Étant donné un graphe connexe H, un graphe *sans-H* est un graphe ne contenant aucune occurrence isomorphe à H. Nous décrivons une méthode générale pouvant être appliquée afin d'énumérer les graphes étiquetés sans H, pour les premiers multicycles, c'est-à-dire, les graphes connexes avec n sommets et $(n+k)$ arêtes pour les premières valeurs de k. Les résultats sont obtenus en prouvant que les fonctions génératrices des structures étudiées vérifient une équation fonctionnelle du type conduction de la chaleur réduisant ainsi l'énumération des graphes sans H à deux nouvelles familles de graphes ; les graphes contenant une seule occurrence de H et ceux en contenant plusieurs mais nécessairement juxtaposées. Par la suite, des méthodes plus générales seront utilisées pour énumérer les premiers multicycles. Bien que difficiles à mettre en oeuvre pour des graphes de grande complexité, ces techniques fournissent les premières réponses pour les graphes dont certains motifs sont interdits. Les méthodes ainsi décrites sont instanciées avec les énumérations des graphes sans triangle et des graphes sans K_4.

1. INTRODUCTION

The graphs to be studied here are labelled and simple, i.e., undirected with labelled vertices, loop-less and without multiple edges. Labelled graph enumeration is important in chemistry and in theoretical physics as discrete models of compounds or clusters. An *H-free* graph is one that does not contain H as a subgraph. Determining the number of graphs with forbidden subgraphs is in general a difficult combinatorial problem (even for "triangle-free" graphs). Various authors have called attention to the lack of results for the simple case of the number of "triangle-free" graphs. The problem was suggested originally by Harary and Palmer in their reference book [6]. The present investigation arises from the need of answers to these questions; the purpose of this paper is to introduce combinatorial methods by which such long-standing problems can be solved even partially for the simpliest cases, e.g., for connected C_3-free graphs with n labelled vertices and $(n+1)$, $(n+2)$ edges or K_4-free graphs with n vertices and $(n+3)$ or $(n+4)$ edges. Note that McKay [15] obtained algorithms that can generate families of combinatorial objects without isomorphs including labelled and unlabelled graphs.

A labelled connected graph can be interpreted as an assembly of distinguishable molecules connected by lines. This physical argument was used by Temperley [1] to find a linear partial differential equation of the heat-conduction type satisfied by the exponential generating functions of connected

This research was done while the first author (V. Ravelomanana) was at LaRIA, Amiens – FRANCE.

labelled graphs. Considerable progress has been made for graphical enumeration and some of it is derived from the concept of random graphs (see, for instance, [3], [4], [8] and [11]) in which successive connections are added at random to an initially disconnected set of n points. Enumeration of labelled graphs according to the number of edges and the number of vertices and the study of random graphs are very close because of the increasing complexity of the successive configurations. A connected component is simple if it is either a tree or unicyclic; the other components are refered to as complex. One can take the difference between the number of vertices and the number of edges as a parameter to count labelled graphs recursively.

Using similar arguments, we obtain here a linear partial differential equation analogous to the one in [1] satisfied by our H-free graphs. In our case, perturbations, which depend linearly only on the enumeration of H, still remain. Consider G_k, an H-free graph chosen at random with n vertices and $n+k$ edges. Adding a new edge randomly to G_k, we obtain a graph G_{k+1}. During the passage from G_k to G_{k+1}, considered as a random graph process, the last edge can change the property H-free of G_k, creating perturbations when counting. These perturbations are due to the possible appearance of forbidden configurations. Mainly two configurations containing H as subgraph can appear with G_{k+1}:

(I) graphs with one and only one occurrence of H
(II) graphs with many occurrences of H but necessarily juxtaposed (the definition of "juxtaposition" will be explained later).

Analytically, these words translate into a differential equation satisfied by our H-free graphs. It reduces our area of investigation considerably and is well suited for the calculus of the generating functions of isomorphism-free graphs. It is linear and leads to a recursion for the generating functions of H-free graphs. But to solve this equation, we have to find the generating functions of families of graphs described above, i.e., (I) and (II). The aim of this paper is to show how to obtain a combinatorial equation satisfied by general H-free graphs and to solve such an equation for the first multicyclic components. Note that in [17] asymptotic estimates of the number of connected H-free graphs are given and used to perform an analysis of random graphs without isomorphic copy of H.

This paper is organized as follows. In section 2, we recall briefly some definitions. Section 3 presents the heat-conduction differential equation in terms of generating functions of H-free graphs according to their complexity. In section 4, combinatorial techniques to count graphs with cutpoints and cutedges are presented (recall that a cutpoint of a graph is one whose removal increases the number of connected components). For our purpose, we can count graphs with some hereditary properties and with cutpoints applying the techniques already presented in [6] or [16]. Similarly, if we denote by a cutedge an edge whose removal increases the number of connected components, we can develop how to enumerate labelled graphs with cutedge(s). For instance, these techniques are used here for some graphs of type (I) and type (II). For the others, we present a possible generalization. In section 5, the method described above is instantiated and we treat the examples of triangle-free connected graphs with n vertices and $(n+1)$ or $(n+2)$ edges or K_4-free connected graphs with n vertices and $(n+3)$ or $(n+4)$ edges.

2. Definitions

We give here some definitions and descriptions of materials which we will encounter throughout this extended abstract.

2.1. **Graph and subgraph.** A *graph* G consists of a set $V = V(G)$ of vertices and a specified set $X = X(G)$ of unordered pairs of distinct points. This excludes self-loops and multiple edges. In a labelled graph of order n (with n vertices), the labels $1, 2, \cdots, n$ are assigned to its vertices. Two labelled graphs G_1 and G_2 are considered *isomorphic* if and only if there is a mapping from $V(G_1)$ to $V(G_2)$ which preserves not only the adjacency but also the labeling of the vertices. A *subgraph* H of a graph G has $V(H) \subseteq V(G)$ and $X(H) \subseteq X(G)$. G is a *supergraph* of H if and only if H is

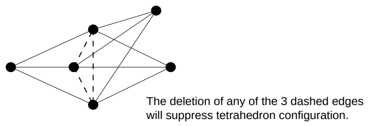

FIGURE 1. 3 tetrahedrons 3-juxtaposed

a subgraph of G. Throughout the rest of this paper (unless specified), H is a given subgraph with $v(H)$ vertices and $e(H)$ edges. Furthermore, h denotes the number of ways to label H.

2.2. **m-juxtaposition.** An *m-juxtaposition* of H is a graph with subgraphs isomorphic to H having *m common edges* such that any deletion of one of these edges will suppress all occurrences of H in the graph. The figure 1 represents an example of a *3-juxtaposition* of tetrahedrons. The word *juxtaposition* will be used in general if we do not consider precisely the number of edges to delete to suppress any configuration of H in some graph G.

2.3. **Generating functions.** *Exponential generating functions* (EGF or simply GF for brief) are suitable for labelled enumeration problems. An EGF of the formal power series $< A_0, A_1, \cdots >$ is $A(z) = \sum_n A_n \frac{z^n}{n!}$. The operator $[z^n]$ applied to the polynomial $P(z)$ yields the coefficient of z^n in $P(z)$. GF can be multivariate. A *bivariate* GF is a mixed exponential GF; $F(w,z) = \sum_{m,n} F_{m,n} w^m \frac{z^n}{n!}$. Throughout this paper, we will use mainly bivariate generating functions, i.e., if $\mathcal{F}$ is a family of graphs, we denote by $F(w,z)$ its bivariate EGF where the variable w marks the edges and the variable z reflects the number of the vertices of the graph of $\mathcal{F}$. The case of rooted labelled trees is a good example of a GF (see [6] for more details). The number of rooted trees of order n is n^{n-1}. Let T be the bivariate GF for labelled trees. The bivariate EGF for rooted trees is given by

$$T(w,z) = \frac{T(wz)}{w} = \sum_{n \geq 1} \frac{(wn)^{n-1} z^n}{n!} . \tag{1}$$

A connected graph G with k edges more than its number of vertices is called a *k-excess* graph. Denote by W_k the EGF of k-excess graphs; Wright [7] computed $W_k(w,z)$ for all $k \geq 1$ (where the variable w, resp. z, reflects the number of edges, resp. vertices). We refer the reader to [11, sect. 10] for the use of derivatives to obtain the series of GF for k-excess graphs.

Let F_k be the GF of labelled k-excess graphs which do not contain H and N_k the GF of labelled k-excess supergraphs of H. Our goal is to find F_k and/or N_k. Let us now give other definitions for our graphs, saving the justification of their uses later. We denote by S_k the GF of k-excess graphs with one and only one occurrence of H and by $J_{k,i}$ the GF of labelled k-excess graphs containing one and only one i-juxtaposition of H. R_k is the GF of k-excess graphs containing many occurrences of H such that one edge-deletion does not suffice to eliminate all occurrences of H in the resulting graph. In other words, R_k is the EGF associated to the rest of labelled connected k-excess graphs not in the families $\mathcal{S}_k$, $\mathcal{J}_k$ and $\mathcal{F}_k$ described above[1].

Throughout this note, we let $T \equiv T(wz)$ and we define by ϑ_x the differential operator $x\frac{\partial}{\partial x}$ (see [12]).

3. RECURRENCES AND GENERATING FUNCTIONS

We have the following theorem relating F_{k+1}, S_{k+1}, J_{k+1} to F_i for $i \in [-1, k]$:

Theorem 1. *Using derivatives with H-free graphs, we have*

$$\vartheta_w F_{k+1} + e(H) S_{k+1} + \sum_{i \geq 1} i\, J_{k+1,i} =$$

[1] the letter "S" stands for single occurrence, "J" is for juxtaposition, "N" is for non H-free and "R" is for the rest

$$w\left(\frac{\vartheta_z^2-\vartheta_z}{2}-\vartheta_w\right)F_k+w\sum_{p+q=k,p\geq q\geq -1}\frac{1}{(1+\partial_{p,q})}\left(\vartheta_z F_p\right)\left(\vartheta_z F_q\right) \tag{2}$$

where $\partial_{p,q}$ is the Kronecker product, F_p and S_p are the GF described in table 1, $e(H)$ is the total number of edges in H, T is the GF for rooted labelled trees given in (1), i is the number of intersecting edges in some i-juxtaposition of configurations of H and $J_{k,i}$ the GF of all i-juxtaposition of configurations of H with k exceeding edges.

Proof. The principle is based upon edge distinction (see also [17]). Consider G_k, a connected graph, with n vertices and $n+k$ edges without occurrence of H, chosen at random and let G_{k+1} be a connected graph obtained from G_k after the addition of an edge. Three cases can appear:

- G_{k+1} is still H-free,
- in G_{k+1}, there is one and only one occurrence of H,
- there are many occurrences of H, i-juxtaposed in G_{k+1}.

On the right side of (2), we distinguish a particular edge in a H-free graph with n vertices and $(n+k+1)$ edges. This edge can be seen as the last added in some graphs with k exceeding edges in order to obtain $(k+1)$-excess graphs. One can do this in two different ways. First, we can choose two distinct vertices which aren't already adjacent to avoid self-loops and/or multiple edges and put an edge between them. This operation correponds analytically to: $w(\frac{{\vartheta_z}^2-\vartheta_z}{2}-\vartheta_w)F_k$. Then, we can join two graphs $G_p\in F_p$ and $G_q\in F_q$ such that $p+q=k$ to build a new graph with $k+1$ edges more than vertices; a compensating factor $\frac{1}{2!}$ appears when $p=q$ due to the symmetry. Note that when $q=-1$, we have $(\vartheta_z F_{-1})(\vartheta_z F_{k+1})=T\,(\vartheta_z F_{k+1})$. But the resulting graph can contain configuration(s) of H as described above. On the left side of (2), an edge can be distinguished in two ways:

- an edge whose removal doesn't change the property "H-free" of our graph,
- an edge whose removal transform our "non H-free" graphs onto "H-free" ones.

We have to add the cases where occurrences of H appear. Working temporarily with trivariate GF; we now add v as a new color to mark edges that can transform our H-free graphs onto supergraphs of H.

In the case where an unique occurrence of H appears, we have

$$\left[v\frac{\partial S_{k+1}(w,v,z)}{\partial v}\right]_{|v=w}=e(H)\times S_{k+1}(w,w,z) \tag{3}$$

where $e(H)$ is the total number of edges in H; because all the edges in this occurrence can be the last one that constitute H. In the case where the occurrences of H are i-juxtaposed, only edges such that their deletions (see figure 1) removes all occurrences of H can be marked with color v and then we have a trivariate GF

$$\left[v\frac{\partial J_{k+1,i}(w,v,z)}{\partial v}\right]_{|v=w}=i\;J_{k+1,i}(w,w,z)\,. \tag{4}$$

Summing over all possible numbers of edges in the intersection of all juxtaposed occurrences of H yields the theorem. □

One of the consequences of (2) is that with the knowledge of $(F_k)_{k\leq n}$ and $S_{k+1},\sum iJ_{k+1,i}$, one can determine F_{k+1}. Since the sum $N_k+R_k=W_k$ is known (see [7, 11]), N_k the GF associated to supergraphs of H can also be determined.

Corollary 2. *Denote respectively by*

- *$S(w,z)$ the GF of all (connected labelled) graphs with one occurrence of H,*
- *$J_i(w,z)$ the GF of graphs with juxtaposed occurrences of H on i common edges*
- *and $F(w,z)$ the GF of H-free graphs.*

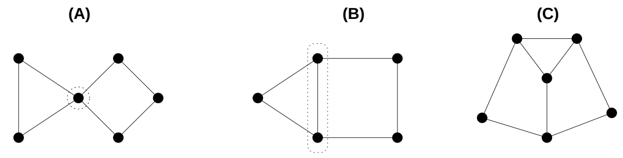

FIGURE 2

Let Φ be the following formal power series

$$\Phi(w,z) = 2\left(e(H)S(w,z) + \sum_{i\geq 1} iJ_i(w,z)\right)\exp\left(F(w,z)\right). \tag{5}$$

Then,

$$\Phi(w,z) = 2w\left(\left(\frac{\vartheta_z^2 - \vartheta_z}{2} - \vartheta_w\right)F(w,z) + \left(\vartheta_z F(w,z)\right)^2\right)\exp\left(F(w,z)\right) \tag{6}$$

and the coefficients of Φ satisfy

$$\forall n \textit{ fixed}, \sum_{m=0}^{\frac{n(n-1)}{2}} \frac{[w^m z^n]\,\Phi(w,z)}{2m\binom{\frac{n(n-1)}{2}}{2}} = 1\,. \tag{7}$$

Proof. If successive edges are added at random to an initially empty n-vertex graph until configuration(s) of H occurs, then the obtained graph consists of a set of H-free connected components and *one* connected component with at least one occurrence of H inside. Thus, in (7), the term $\frac{1}{2m}\binom{\frac{n(n-1)}{2}}{2}^{-1}$ represents a probabilistic weighting for each value of m, where m is the number of edges necessary to add until the first occurrence of H appears (see [8] or [11]). □

4. Cutpoints, cutedges, semi-chromatic H-free graphs and GF

In this section, we consider connected graphs with one and only one occurrence of H. Note that if $H^{'}$ represents any juxtaposition of H, we can work directly in the same manner as with single occurrence of $H^{'}$. We can subdivide graphs containing an occurrence of H in 3 types (A), (B) and (C) as in the figure 2 where H is represented by a triangle. The first two types (A) and (B) of figure 2 can be described as follows; (A) represents the "concatenation" of two graphs N and F (respectively non-H-free and H-free) by a common vertice. In the figure, N is simply a triangle. This is refered here as a serial composition of graphs. (B) is the "concatenation" of the same graphs but by a common edge and their two incident vertices. We refer this concatenation here as parallel composition of graphs. The type (C) of figure 2 represents one of the graphs not in (A) nor in (B).

4.1. The serial composition or concatenation by a vertex.

As already stated, a cutpoint of a graph is one whose removal increases the number of components. Since a graph with one cutpoint may be considered to be rooted at the cutpoint, the number of connected graphs with one cutpoint can be expressed in terms of the GF of the k different blocks, $B_1, B_2, ..., B_k$ each one rooted at the same cutpoint (cf. [6] or [16]). This technique can be applied to count certain configurations.

Lemma 1. *If we have two graphs joined by a common vertex, with on one side an H-free graph F and on the other side a supergraph of H, called N, then the number of ways to label such concatenation of two graphs is*

$$\left[\frac{1}{z}\frac{1}{(1-wz)}\left(z\frac{\partial}{\partial z}\underline{F}(w,z)\right)\left(z\frac{\partial}{\partial z}\underline{N}(w,z)\right)\right]_{|wz=T} \tag{8}$$

where $\underline{F}$ (resp. $\underline{N}$) is the GF for smooth graphs (graphs with no vertices of degree 1) of F (resp. of N).

Proof. This is the combination of the approach presented in [16] and Wright's reduction method [7]. We have to introduce a factor $\frac{1}{z}$ to relabel the common cutpoint considered here as special. We insert the term $\frac{1}{1-wz}$ to represent a possible bridge, i.e., a sequence of vertices of degree 2 except the two extremal ones, between the two sides N and F. With the substitution $T \equiv T(wz)$ for each occurrence of wz, we reverse the *vertexectomy* process starting with a smooth graph and sprout rooted trees from each node. □

4.2. **The parallel composition or concatenation by an edge.** Graphs of the type represented by the figure 2 (B) can be enumerated in an analogous way.

Lemma 2. *If we have two graphs joined by a common edge, the number of ways to label such graph is*

$$\left[\frac{2}{wz^2}\left(z\frac{\partial}{\partial z}\underline{F}(w,z)\right)\left(z\frac{\partial}{\partial z}\underline{N}(w,z)\right)\right]_{|wz=T} \tag{9}$$

where $\underline{F}$ (resp. $\underline{N}$) is the GF for smooth graphs of F (resp. of N).

Proof. The formula in (9) differs slightly from those in (8). The factor $\frac{2}{wz^2}$ comes from the fact that we have in figure 2 (B) a common edge which is defined by his two common vertices and can be seen as a root-edge. A graph represented by the figure 2 (B) can be considered as pendant to this edge. □

4.3. **Labelled and semi-chromatic graphs.** The two techniques presented above suggest a generalization. A second kind of marking is considered here. Each vertex is given one label and one color which is familiar from graph coloring and receive considerable amount of attention in combinatorics. Given a set of colors $\{c_1, c_2, ..., c_k\}$, a *labelled chromatic* graph is subject to the condition that adjacent vertices may not have the same color c_i. Riordan derived a formula for chromatic trees [2]. Given a predefined set of colors $\{c_1, c_2, ..., c_k\}$ and a special color c_0 which we call here the *neutral color*, a labelled graph G is *semi-chromatic* iff

- some vertices of G are colored with the neutral color c_0 the others are colored with colors in $\{c_1, c_2, ..., c_k\}$,
- for each connected component of G, at least one vertex is colored with one of the colors c_i, $1 \le i \le k$
- the vertices colored with $c_i, 1 \le i \le k$ are subject to the chromatic condition, i.e two adjacent vertices may not have the same color c_i if $1 \le i \le k$. The vertices colored with the neutral color c_0 are free.

As already remarked, the number of triangle-free graphs can be deduced from the number of graphs with one triangle or with juxtaposition of triangles. In this paragraph, we will show that these enumerations are in their turn equivalent to that of semi-chromatic labelled triangle-free graphs with 3 principal colors and 1 neutral. This is a consequence of the method described in [14] where significant examples are also given. Let us recall briefly Bagaev's *shrinking-and-expanding* method. In order to enumerate graphs of a given type, an induced subgraph with special properties should be chosen and shrunk to a *marked* vertex.

Separately, we have to calculate:

- the number of the obtained graphs, rooted at a fixed vertex of degree d,
- the number of the shrunk subgraphs,
- the number of ways to reconstruct the initial graphs.

Then, the number of the initial graphs is the sum, over all possible degrees of the fixed vertex, of the products of the 3 numbers described above. For our purpose, the shrinking-and-expanding method can be very useful as we want to enumerate graphs with one occurrence of given subgraph (H or l-juxtaposition of H, especially when H is a triangle). Let us apply the Bagaev's method with connected graphs containing exactly one triangle. If we shrink the triangle, we have a graph rooted at a special vertex of degree d. Then, two cases can occur after the shrinking process

1- the obtained graph contains triangle(s)
2- there are no more triangles in the obtained graph.

In the latter case, the number of ways to reconstruct graphs with exactly a triangle are simply 3^d. In the first case, we have to avoid building another triangles during the reconstruction.

Lemma 3. *Denote by $\chi_3(w,z)$ the exponential generating function of semi-chromatic labelled triangle-free graphs with 3 significant colors and 1 neutral color. Then, we have*

$$S(w,z) = \frac{T^3}{6}\chi_3(w,z) \tag{10}$$

where $T(w,z)$ is GF for Cayley's rooted trees and $S(w,z)$ is the GF for connected labelled graphs with exactly one occurrence of a triangle.

Note that χ_3 contains general (connected or not) triangle-free graphs. The fact that they are semi-chromatic ensures that in each connected component of χ_3 at least one vertex is colored (cf. definition of semi-chromatic).

Proof. Clearly, the number of such reconstructions is the number of ways to put 3 colors, which we call a, b and c, as second kind of marking on some of the vertices of triangle-free graphs such that no two adjacent vertices may have the same color a,b or c in order to have one and only one triangle. Thus, there are $\binom{n}{3}$ ways to distinguish the 3 colors, i.e., to label the root-triangle. And for each labelled triangle-free graph, we have to choose arbitrarily the number of vertices to be colored or to be attached to these 3 distinguished labels. If two adjacent vertices are chosen, they have to be attached to two distinct vertices of the root-triangle. This is equivalent to the number of semi-chromatic triangle-free graphs using 3 significant colors. Then, we simply replace the 3 vertices a, b and c of the triangle with labelled rooted trees which are given by $T(w,z)$. □

5. Instantiations

In this section, we give some examples to illustrate and apply the methods presented previously. To avoid confusion, if we are seeking H-free graphs, we will denote by $F_{k,H}$ the GF of H-free graphs having k-excess. The second index represents simply the forbidden subgraph. The same remark holds for $S_{k,H}$ or $J_{k,H}$. The first example is the enumeration of triangle-free or C_3-free graphs.

5.1. Triangle-free graphs.

The generating function $W_0(w,z)$ for unicyclic components is[2]

$$W_0(w,z) = \frac{1}{2}\ln\frac{1}{1-T} - \frac{T}{2} - \frac{T^2}{4}. \tag{11}$$

The GF for unicyclic graphs without triangle is simply

$$F_{0,C_3}(w,z) = W_0(w,z) - \frac{T^3}{6} = \frac{1}{2}\ln\frac{1}{1-T} - \frac{T}{2} - \frac{T^2}{4} - \frac{T^3}{6}. \tag{12}$$

The GF for graphs containing one and only one triangle and having one excess, $S_{1,C_3}(w,z)$, can be derived using the principles given by lemmas 1, 2 and we obtain

$$S_{1,C_3}(w,z) = w\frac{T^5}{4}\frac{(2-T)}{(1-T)^2}. \tag{13}$$

Using again (9), we have the GF for 1-juxtaposition of 2 triangles, denoted here $J_{1,C_3}(w,z)$

$$J_{1,C_3}(w,z) = \frac{1}{2!}w\frac{T^5}{2}. \tag{14}$$

[2]Recall that we use the notation $T \equiv T(wz)$ for sake of simplicity and for each GF, the variable w (resp. z) marks the edges (resp. vertices)

The factor $\frac{1}{2!}$ arises from the global symmetry of the 2 juxtaposed triangles. The GF for triangle-free graphs having 1 excess, $F_{1,C_3}(w,z)$ is derived from formulae (12), (13), (14) and (2), namely

$$F_{1,C_3}(w,z) = w\frac{T^5}{24}\frac{(2+6T-3T^2)}{(1-T)^3}\,. \tag{15}$$

For graphs having 2 excesses, the removal of all edges and vertices by the Wright's reduction method leads to the set of graphs represented by figure 3 for graphs containing 1 triangle and figure 4 for graphs with juxtaposition of triangles. Given a family $\mathcal{F}$ of graphs, we denote by $\underline{F}$ the EGF of smooth elements of $\mathcal{F}$. For triangle-free graphs we have from (15)

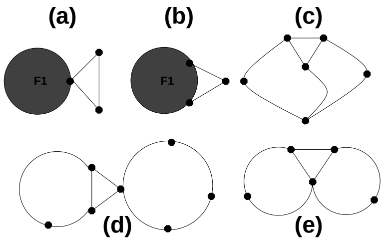

FIGURE 3. Basic 2-excess graphs with one triangle.

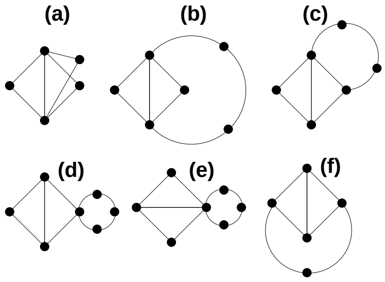

FIGURE 4. 2-excess graphs with a juxtaposition of triangles.

$$\underline{F_{1,C_3}}(w,z) = w\frac{w^5z^5}{24}\frac{(2+6wz-3w^2z^2)}{(1-wz)^3} \tag{16}$$

Then, the application of the lemmas 1 and 2 to figure 3 (a) and 3 (b) gives

$$\left[w^2 z\vartheta_w\left(\underline{F_{1,C_3,}}(w,z)\right) + \frac{w^3z^2}{2(1-wz)}\vartheta_z\left(\underline{F_1}(w,z)\right)\right]_{|wz=T}\,. \tag{17}$$

Figures 3 (c), 3 (d) and 3 (e) give respectively

$$w^2\frac{T^6}{6}\frac{(3-2T)}{(1-T)^3} + \frac{w^2T^7}{2(1-T)^2} + \frac{w^2T^8}{4(1-T)^3}\,. \tag{18}$$

Summing (17) and (18), one can deduce

$$S_{2,C_3}(w,z) = \frac{w^2T^6}{48}\frac{(48+18T-140T^2+119T^3-30T^4)}{(1-T)^5}\,. \tag{19}$$

The figure 4 represents the basic 2-excess graphs with juxtapositions of triangles. The corresponding GF of figure 4 is

$$\begin{aligned} J_{2,C_3}(w,z) \quad = \quad & \left[\underbrace{\frac{w}{z(1-wz)}\vartheta_z\left(\frac{w^5z^4}{4}\right)\vartheta_z\left(F_{0,s}(w,z)\right)}_{\text{figures 4 (d), (e)}} + \underbrace{\frac{2}{wz^2}\vartheta_w\left(\frac{w^5z^4}{4}\right)\vartheta_w\left(F_{0,s}(w,z)\right)}_{\text{figures 4 (b), (c)}}\right]_{|wz=T} \\ & + \quad \underbrace{w^2\frac{T^5}{2!3!}}_{\text{for figure 4 (a)}} \quad + \quad \underbrace{w^2\frac{T^5}{4(1-T)}}_{\text{for figure 4 (f)}} \end{aligned}$$

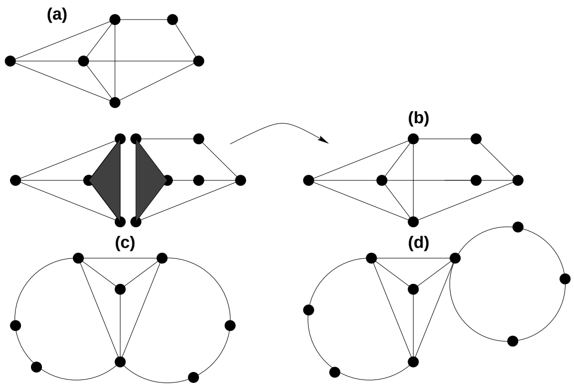

FIGURE 5. Basic graphs with an occurrence of K_4.

It comes

$$J_{2,C_3}(w,z) = \frac{w^2T^5}{6}\frac{(2+5T-4T^2)}{(1-T)^2}\,. \tag{20}$$

The GF of triangle-free graphs is the obtained with (19), (20) and (2)

$$F_{2,C_3}(w,z) = w^2\frac{T^6}{48}\frac{(7+36T-18T^2-40T^3+40T^4-10T^5)}{(1-T)^6}\,. \tag{21}$$

5.2. ***K_4*-free graphs.** If $k<2$ a connected graph with n vertices and $n+k$ edges is K_4-free. The number of 2-excess K_4-free labelled graphs is simply

$$F_{2,K_4}(w,z) = W_2(w,z) - w^2\frac{T^4}{4!}\,. \tag{22}$$

Denote by $F_{0,s}(w,z) = \frac{1}{2}ln\big(\frac{1}{(1-wz)}\big) - \frac{wz}{2} - \frac{w^2z^2}{4}$, the GF for smooth unicyclic graphs, the number of 3-excess graphs with one occurrence of K_4 can be derived using lemmas 1 and 2

$$S_{3,K_4}(w,z) = \left[\,\Big(\frac{2}{wz^2}\vartheta_w\big(\frac{w^6z^4}{24}\big)\vartheta_w\big(\underline{F_0}(w,z)\big) + \frac{1}{z(1-wz)}\underline{F_0}(w,z)\Big)\right]_{|wz=T}\,. \tag{23}$$

There is no possible juxtaposition of K_4 until the number of edges attains $n+4$, then we have

$$J_{4,K_4}(w,z) = \frac{1}{2!}\frac{w^4T^5}{6}\,. \tag{24}$$

In formula (24), the term $\frac{1}{2!}$ reflects the symmetry between the 2 tetrahedrons. With each tetrahedron enumerated by $\frac{w^6z^4}{24}$, we have to choose one face defined by 3 labelled vertices. The relabeling of the common face introduces a factor $\frac{3!}{w^3z^3}$ (as in lemma 2, the common edge introduces a factor $\frac{2}{wz^2}$). (24) is equivalent to

$$\left[\frac{1}{2!}\frac{6}{w^3z^3}\big(4\times\frac{w^6z^4}{24}\big)^2\right]_{|wz=T}\,. \tag{25}$$

The enumeration of 4-excess graphs with one occurrence of K_4 is very similar to that of 1-excess graphs with one occurrence of C_3. The figure below shows all basic 4-excess graphs with 1 K_4

Figure 5 (b) is the "concatenation" of the 2 graphs on his left. It can be derived as we did for (25)

$$\left[\frac{6}{w^3z^3}4\left(\frac{1}{24}w^6z^4\right)\left(\frac{w^8z^6}{6}\frac{(3-2wz)}{(1-wz)^3}\right)\right]_{|wz=T}\,. \tag{26}$$

The GF corresponding to figures 5 (a), (c) and (d) are respectively the formulae (27), (27) and (29) given below

$$\frac{w^4T^6}{2(1-T)}\,, \tag{27}$$

$$\left[\frac{1}{2!}\frac{2}{wz^2}\frac{5}{4}\frac{w^8z^4}{(1-wz)}\vartheta_w\left(\underline{F_0}(w,z)\right)\right]_{|wz=T} \tag{28}$$

and

$$\left[\frac{1}{z(1-wz)}2\times\frac{1}{4}\frac{w^8z^4}{(1-wz)}\vartheta_z\left(\underline{F_0}(w,z)\right)\right]_{|wz=T}\,. \tag{29}$$

In total, we have

$$S_{4,K_4}(w,z)=\frac{w^4T^6}{144}\frac{(252-570T+490T^2-181T^3+24T^4}{(1-T)^5}\,. \tag{30}$$

Using (30), (24) and (2), the number of 4-excess labelled graphs not containing K_4 is given by

$$\begin{aligned} F_{4,K_4}(w,z) \quad = \quad & \tfrac{w^4T^6}{11\,520(1-T)^{12}}\times\big(22\,992+177\,504T-671\,536T^2+1\,594\,248T^3 \\ & -2\,547\,280T^4+2\,857\,633T^5-2\,267\,589T^6+1\,262\,986T^7 \\ & -480\,188T^8+117\,520T^9-16\,400T^{10}+960T^{11}\big)\,. \end{aligned} \tag{31}$$

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