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GRAPH WEIGHTS ARISING FROM STATISTICAL MECHANICS

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Abstract. In statistical mechanics it is well known that the coefficients of the virial expansion for a non-ideal gas are computed using the Mayer weight of 2-connected graphs. We study the Second Mayer weight $w_M(c)$ and the Ree–Hoover weight $w_{RH}(c)$ of a 2-connected graph c which arise from the hard-core continuum gas in one dimension. These weights are computed using signed volumes of convex polytopes naturally associated with the graph c. Our results are new formulas of Mayer weights and Ree–Hoover weights for special infinite families of 2-connected graphs.

Résumé. En mécanique statistique, il est bien connu que les coefficients du développement du viriel pour un gaz non-idéal sont calculés en utilisant le poids de Mayer des graphes 2-connexes. Nous étudions le second poids de Mayer $w_M(c)$ et de Ree–Hoover $w_{RH}(c)$ d'un graphe 2-connexe c dans le cas d'un gaz à noyaux durs en dimension un. Ces poids sont calculés à partir des volumes signés de polytopes convexes associés naturellement au graphe c. Nous donnons des nouvelles formules pour le poids de Mayer et de Ree–Hoover pour des familles spéciales infinies de graphes 2-connexes.

1. Introduction

In the present paper, we study *Graph weights* in the context of a non-ideal gas in a vessel $V \subseteq \mathbb{R}^d$. In this case, the *Second Mayer weight* $w_M(c)$ of a connected graph c, over the set $[n] = \{1, 2, \ldots, n\}$ of vertices, is defined by (see [5, 8, 9, 12])

$$w_M(c) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in c} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_{n-1}}, \quad \overrightarrow{x_n} = 0, \tag{1}$$

where $\overrightarrow{x_1}, \ldots, \overrightarrow{x_n}$ are variables in $\mathbb{R}^d$ representing the positions of n particles in V ($V \to \infty$), the value $\overrightarrow{x_n} = 0$ being arbitrarily fixed, and where $f = f(r)$ is a real-valued function associated with the pairwise interaction potential of the particles, see [21, 12].

Let $\mathcal{C}[n]$ be the set of connected graphs over $[n]$. The total sum of weights of connected graphs over $[n]$ is denoted by

$$|\mathcal{C}[n]|_{w_M} = \sum_{c\in\mathcal{C}[n]} w_M(c). \tag{2}$$

The interest of this sequence in statistical mechanics comes from the fact that the pressure P of the system is given by its exponential generating function as follows (see [12]):

$$\frac{P}{kT} = \mathcal{C}_{w_M}(z) = \sum_{n\geq 1} |\mathcal{C}[n]|_{w_M} \frac{z^n}{n!}, \tag{3}$$

where k is a constant, T is the temperature and z is a variable called the *fugacity* or the *activity* of the system. It is known that the weight w_M is multiplicative over 2-connected components so that, in order to compute the weights $w_M(c)$ of the connected graphs $c \in \mathcal{C}[n]$, it is sufficient to compute the weights $w_M(b)$ for 2-connected graphs $b \in \mathcal{B}[n]$ ($\mathcal{B}$ for *blocks*). These occur in the so-called *virial expansion* proposed by Kamerlingh Onnes in 1901

$$\frac{P}{kT} = \rho + \beta_2\rho^2 + \beta_3\rho^3 + \cdots, \tag{4}$$

where ρ is the density. Indeed, it can be shown that

$$\beta_n = \frac{1-n}{n!}|\mathcal{B}[n]|_{w_M}, \tag{5}$$

where $\mathcal{B}[n]$ denotes the set of 2-connected graphs over $[n]$ and $|\mathcal{B}[n]|_{w_M}$ is the total sum of weights of 2-connected graphs over $[n]$. In order to compute this expansion numerically, Ree and Hoover [15] introduced a modified weight denoted by $w_{RH}(b)$, for 2-connected graphs b, which greatly simplifies the computations. It is defined by

$$w_{RH}(b) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|) \prod_{\{i,j\}\notin b} \overline{f}(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1}\cdots d\overrightarrow{x_{n-1}}, \quad \overrightarrow{x_n} = 0, \tag{6}$$

where $\overline{f}(r) = 1 + f(r)$. Using this new weight, Ree and Hoover [15, 16, 17] and later Clisby and McCoy [2, 3] have computed the virial coefficients β_n, for n up to 10, in dimensions $d \leq 8$, in the case of the hard-core continuum gas, that is, when the interaction is given by

$$f(r) = -\chi(r < 1), \quad \overline{f}(r) = \chi(r \geq 1), \tag{7}$$

where χ denotes the characteristic function ($\chi(P) = 1$, if P is true and 0, otherwise).

The main goal of the present paper is to give new explicit formulas for the Mayer and Ree–Hoover weights of certain infinite families of graphs in the context of the hard core continuum gas, defined by (7), in dimension $d = 1$. The values $w_M(c)$ and $w_{RH}(c)$ for all 2-connected graphs c of size at most 8 are given in [5, 6]. In Section 2, we give explicit linear relations expressing the Ree–Hoover weights in terms of the Mayer weights and vice versa. The total Mayer weight $|\mathcal{B}[n]|_{w_M}$ is then rewritten in terms of the weight function w_{RH} introduced by Ree and Hoover [15, 16]. The interest of using the Ree–Hoover weight is that it has the value zero for many graphs. Section 3 is devoted to the special case of the hard-core continuum gas in one dimension in which the Mayer weight turns out to be a signed volume of a convex polytope $\mathcal{P}(c)$ naturally associated with the graph c. A decomposition of the polytope $\mathcal{P}(c)$ into a certain number of simplices is exploited. This method was introduced in [12] and was adapted in [5, 9] to the context of Ree–Hoover weights and is called the method of graph homomorphisms. The explicit computation of Mayer or Ree–Hoover weights of particular graphs is very difficult in general and has only been made for certain specific families of graphs (see [7, 8, 9, 10, 11, 12]). In the present paper we extend this list to other graphs. We give new explicit formulas of the Ree–Hoover weight of these graphs in Section 4. Section 5 is devoted to the explicit computation of their Mayer weight. The following conventions are used in the present paper. Each graph g is identified with its set of edges. So that, $\{i, j\} \in g$ means that $\{i, j\}$ is an edge in g between vertex i and vertex j. The number of edges in g is denoted by $e(g)$. If e is an edge of g (i.e., $e \in g$), $g\backslash e$ denote the graph obtained from g by removing the edge e. If b and d are graphs, $b \subseteq d$ means that b is a subgraph of d. The complete graph on the vertex set $[n] = \{1, 2, \ldots, n\}$ is denoted by K_n. The complementary graph of a subgraph $g \subseteq K_n$ is the graph $\overline{g} = K_n\backslash g$.

2. Relations between Mayer weight and Ree–Hoover weight

An important rewriting of the virial coefficients was performed by Ree and Hoover [15, 16] by introducing the function

$$\overline{f}(r) = 1 + f(r) \tag{8}$$

and defining a new weight (denoted here by $w_{RH}(b)$) for 2-connected graphs b, by (9)

$$w_{RH}(b) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|) \prod_{\{i,j\}\notin b} \overline{f}(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1}\cdots d\overrightarrow{x_{n-1}}, \quad \overrightarrow{x_n} = 0, \tag{9}$$

and then expanding each weight $w_M(b)$ by substituting $1 = \overline{f} - f$ for pairs of vertices not connected by edges. Upon performing this rewriting of the Mayer weight series, vertices in the resulting graphs will all be mutually connected by either f bonds (solid lines) or $\overline{f}$ bonds (dotted lines). In general, using Möbius inversion, it is easy to state formulas linking the two weights w_M and w_{RH}. These formulas are implicit in [16].

Proposition 1 ([9]). *For a 2-connected graph b, we have*

$$w_{RH}(b) = \sum_{b \subseteq d \subseteq K_n} w_M(d), \tag{10}$$

$$w_M(b) = \sum_{b \subseteq d \subseteq K_n} (-1)^{e(d)-e(b)} w_{RH}(d). \tag{11}$$

Proof. See [9]. □

Consequently, the virial coefficient can be rewritten in the form

$$\beta_n = \frac{1-n}{n!} \sum_{b \in \mathcal{B}[n]} a_n(b) w_{RH}(b), \tag{12}$$

for appropriate coefficients $a_n(b)$ called the *star content* of the graph b. The importance of (12) is due to the fact that $a_n(b) = 0$ or $w_{RH}(b) = 0$ for many graphs b. This greatly simplifies the computation of β_n.

Using the definition of the Ree–Hoover weight, we have

$$w_{RH}(K_n) = w_M(K_n), \quad n \geq 2. \tag{13}$$

3. Hard-core continuum gas in one dimension

Consider n hard particles of diameter 1 on a line segment. The *hard-core* constraint translates into the interaction potential φ, with $\varphi(r) = \infty$, if $r < 1$, and $\varphi(r) = 0$, if $r \geq 1$, and the Mayer function f and the Ree–Hoover function $\overline{f}$ are given by (7). Hence, we can write the Mayer weight function $w_M(c)$ of a connected graph c as

$$w_M(c) = (-1)^{e(c)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\} \in c} \chi(|x_i - x_j| < 1) dx_1 \dots dx_{n-1}, \qquad x_n = 0, \tag{14}$$

and the Ree–Hoover's weight function $w_{RH}(c)$ of a 2-connected graph c as

$$w_{RH}(c) = (-1)^{e(c)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\} \in c} \chi(|x_i - x_j| < 1) \prod_{\{i,j\} \notin c} \chi(|x_i - x_j| > 1) dx_1 \dots dx_{n-1}, \tag{15}$$

with $x_n = 0$ and where $e(c)$ is the number of edges of c. Note that $w_M(c) = (-1)^{e(c)} \mathrm{Vol}(\mathcal{P}(c))$, where $\mathcal{P}(c)$ is the polytope defined by

$$\mathcal{P}(c) = \{X \in \mathbb{R}^n : x_n = 0, |x_i - x_j| < 1 \text{ for all } \{i,j\} \in c\} \subseteq \mathbb{R}^{n-1} \times \{0\} \subseteq \mathbb{R}^n,$$

where $X = (x_1, \dots, x_n)$. Similarly, $w_{RH}(c) = (-1)^{e(c)}\mathrm{Vol}(\mathcal{P}_{RH}(c))$, where $\mathcal{P}_{RH}(c)$ is the union of polytopes defined by

$$\mathcal{P}_{RH}(c) = \{X \in \mathbb{R}^n : x_n = 0,\ |x_i - x_j| < 1 \text{ for all } \{i,j\} \in c, \\ |x_i - x_j| > 1 \text{ for all } \{i,j\} \in \overline{c}\} \subseteq \mathbb{R}^{n-1} \times \{0\} \subseteq \mathbb{R}^n.$$

3.1. **Sufficient conditions for $w_{RH} = 0$.** When the Ree–Hoover transformation is made, many graphs have zero star content and hence do not contribute to the virial coefficient. In addition, some Ree–Hoover graph weights may be zero for geometrical reasons. We found sufficient conditions for families of graphs which guarantee the vanishing of their Ree–Hoover weights (see [5]). We introduce first some variants of the notion of subgraph and then state an associated lemma.

Definition 2. *Let g be a simple graph on the vertex set U and g' be a subgraph of g on the vertex set $U' \subseteq U$. The graph g' is said to be* induced *by g if*

$$g' = g \cap K_{U'}, \tag{16}$$

where $K_{U'}$ is the complete graph on U'. If a graph h is isomorphic to an induced subgraph of g, we write $h \mathrel{\overline{\subseteq}} g$.

Proposition 3 ([9])**.** *Let g and h be two 2-connected graphs. In the case of hard-core continuum gas in one dimension, we have*

$$h \mathrel{\overline{\subseteq}} g \quad \text{and} \quad w_{RH}(h) = 0 \quad \text{imply} \quad w_{RH}(g) = 0. \tag{17}$$

Proof. See [9]. □

Theorem 4 ([9])**.** *The Ree–Hoover weight of a 2-connected graph g of size n is zero if g satisfies one of the following conditions:*

$$g \textit{ is chordal}:\ C_k \mathrel{\overline{\subseteq}} g, \quad k \geq 4, \tag{18}$$

$$\text{or } g \textit{ is claw-free}:\ S_3 \mathrel{\overline{\subseteq}} g, \tag{19}$$

where S_3 is the 3-star graph (see Figure 1) and C_k is the cycle on k elements.

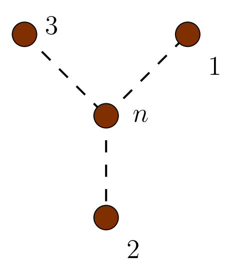

FIGURE 1. The graph S_3

Proof. See [9]. □

3.2. **Graph homomorphisms.** The method of graph homomorphisms was introduced by Labelle, Leroux and Ducharme [12] for the exact computation of the Mayer weight $w_M(b)$ of an arbitrary 2-connected graph b in the context of hard-core continuum gas in one dimension and was adapted by Kaouche and Leroux [5, 9] to the context of Ree–Hoover weights. Since $w_M(b) = (-1)^{e(b)}\mathrm{Vol}(\mathcal{P}(b))$, the computation of $w_M(b)$ is reduced to the computation of the volume of the polytope $\mathcal{P}(b)$ associated with b. In order to evaluate this volume, the polytope $\mathcal{P}(b)$ is decomposed into $\nu(b)$ simplices which are all of volume $1/(n-1)!$. This yields $\mathrm{Vol}(\mathcal{P}(b)) = \nu(b)/(n-1)!$. The simplices are encoded by a diagram associated with the integral parts and the relative positions of the fractional parts of the coordinates $x_1, \dots, x_n$ of points $X \in \mathcal{P}(b)$.

More precisely, with each real number x, they associate an ordered pair (ξ_x, h_x), called the fractional representation of x, where $h_x = \lfloor x \rfloor$ is the integral part of x and $\xi_x = x - h_x$ is the (positive) fractional part of x, so that $x = \xi_x + h_x$. Then, for $x \neq y$, the condition $|x-y| < 1$ translates into "assuming $\xi_x < \xi_y$, then $h_x = h_y$ or $h_x = h_y + 1$". Geometrically, the slope of the line segment between the points (ξ_x, h_x) and (ξ_y, h_y) in the plane should be either zero or negative. Now consider a 2-connected graph b with vertex set $V = [n] = \{1, 2, \dots, n\}$, and let $X = (x_1, \dots, x_n)$ be a point in the polytope $\mathcal{P}(b)$. Let us write (ξ_i, h_i) for the fractional representation of the coordinate x_i of X, $i = 1, \dots, n$. For $x_n = 0$, it will be convenient to use the special representation $\xi_n = 1.0$ and $h_n = -1$. The volume of $\mathcal{P}(b)$ is not changed by removing all hyperplanes $\{x_i - x_j = k\}$, for $k \in \mathbb{Z}$. Hence, we can assume that all the fractional parts ξ_i are distinct. We form a subpolytope of $\mathcal{P}(b)$ by keeping the "heights" $h_1, h_2, \dots, h_n$ fixed as well as the relative positions (total order) of the fractional parts $\xi_1, \xi_2, \dots, \xi_n$. Let $h : V \to \mathbb{Z}$ denotes the height function $i \mapsto h_i$ and $\beta : V \to [n]$ be the permutation of $[n]$ for which $\beta(i)$ gives the rank of ξ_i in this total order. Note that $\beta(n) = n$. The corresponding simplex will be denoted by $\mathcal{P}(h, \beta)$. Explicitly, each simplex can be written as

$$\mathcal{P}(h,\beta) = \{(h_1+\xi_1, \dots, h_{n-1}+\xi_{n-1}, 0) : 0 < \xi_{\beta^{-1}(1)} < \dots < \xi_{\beta^{-1}(n-1)} < 1\}, \quad (20)$$

and it is shown in [12] (see also [5] for more details) that each such simplex is affine-equivalent (with Jacobian 1) to the standard simplex

$$\mathcal{P}(0, \mathrm{id}) = \{(\xi_1, \xi_2, \dots, \xi_{n-1}, 0) : 0 < \xi_1 < \xi_2 < \dots < \xi_{n-1} < 1\}$$

in $\mathbb{R}^{n-1} \times \{0\}$, of volume $1/(n-1)!$.

Note that the simplices (20) are disjoint and each such simplex can be characterized by its centre of gravity

$$X_{h,\beta} = (h_1 + \frac{\beta(1)}{n}, h_2 + \frac{\beta(2)}{n}, \dots, h_{n-1} + \frac{\beta(n-1)}{n}, 0) \in \mathbb{R}^{n-1} \times \{0\}.$$

Note also that, when there are no restrictions on h and β, the union of the closed simplices $\overline{\mathcal{P}(h,\beta)}$ coincides with the whole configuration space $\mathbb{R}^{n-1} \times \{0\}$.

Using the fractional coordinates to represent the centre of gravity $X_{h,\beta}$ of the simplex $\mathcal{P}(h,\beta)$, and drawing a line segment connecting $x_i = (h_i, \xi_i)$ and $x_j = (h_j, \xi_j)$ for each edge $\{i,j\}$ of the graph b, we obtain a configuration in the plane which can be seen as an homomorphic image of b which characterizes the subpolytope $\mathcal{P}(h,\beta)$. For example, take $n = 6$ and $b = \{\{1,3\},\{1,5\},\{1,6\},\{2,3\},\{2,4\},\{5,6\}\}$. Figure 2 illustrates the corresponding configuration, where the homomorphic image of b appears clearly. The next proposition summarizes the above discussion.

Proposition 5 ([12]). *Let b be a 2-connected graph with vertex set $V = [n]$, and consider a function $h : V \to \mathbb{Z}$ and a bijection $\beta : V \to [n]$ satisfying $\beta(n) = n$. Then the simplex $\mathcal{P}(h,\beta)$ corresponding to the pair (h,β) is contained in the polytope $\mathcal{P}(\beta)$ if and only if the following condition is satisfied:*

$$\text{for any edge } \{i,j\} \text{ of } b, \quad \beta(i) < \beta(j) \quad \text{implies} \quad h_i = h_j \text{ or } h_i = h_j + 1. \tag{21}$$

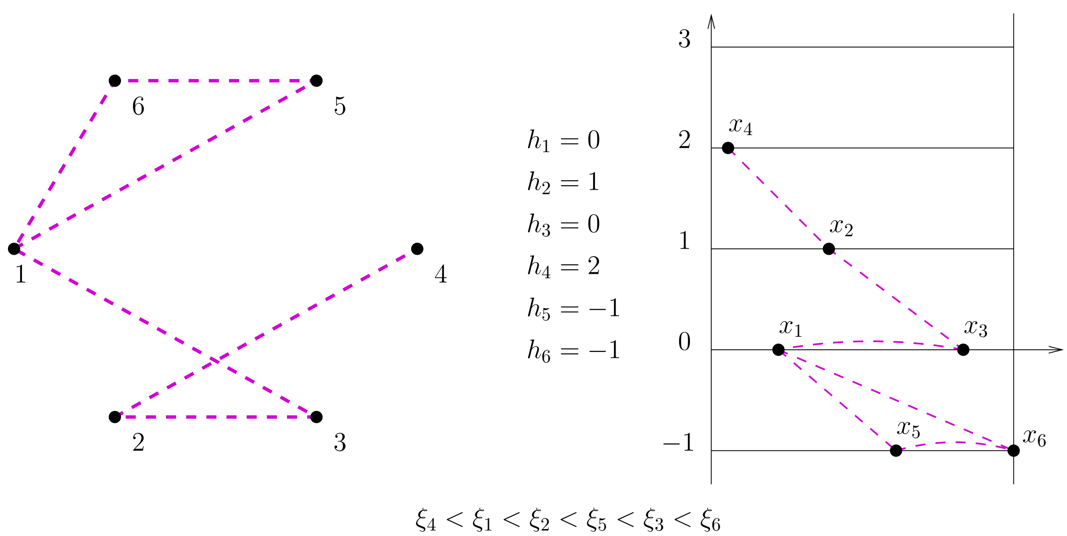

FIGURE 2. Fractional representation of a simplicial subpolytope of a graph b

Corollary 6 ([12]). *Let b be a 2-connected graph and let $\nu(b)$ be the number of pairs (h,β) such that the condition (21) is satisfied. Then the volume of the polytope $\mathcal{P}(b)$ is given by*

$$\mathrm{Vol}(\mathcal{P}(b)) = \nu(b)/(n-1)!. \tag{22}$$

Proposition 6 can be used to compute the weight of some families of graphs, since $w_M(b) = (-1)^{e(b)}\mathrm{Vol}(\mathcal{P}(b))$.

In a similar fashion we can adapt the above configurations to the context of the Ree–Hoover weight.

Proposition 7 ([9])**.** *Let b be a 2-connected graph with vertex set $V = [n]$, and consider a function $h : V \to \mathbb{Z}$ and a bijection $\beta : V \to [n]$ satisfying $\beta(n) = n$. Then the simplex $\mathcal{P}(h, \beta)$ corresponding to the pair (h, β) is contained in the polytope $\mathcal{P}_{RH}(b)$ if and only if the following conditions are satisfied:*

$$\text{for any edge } \{i, j\} \text{ of } b, \quad \beta(i) < \beta(j) \quad \text{implies} \quad h_i = h_j \text{ or } h_i = h_j + 1, \tag{23}$$

$$\text{for any edge } \{i, j\} \text{ of } \overline{b}, \quad \beta(i) < \beta(j) \quad \text{implies} \quad h_i \le h_j - 1 \text{ or } h_i \ge h_j + 2. \tag{24}$$

Proof. See [9]. □

Proposition 8 ([9])**.** *Let b be a 2-connected graph and let $\nu_{RH}(b)$ be the number of pairs (h, β) such that conditions* (23) *and* (24) *are satisfied. Then the volume of $\mathcal{P}_{RH}(b)$ is given by*

$$\mathrm{Vol}(\mathcal{P}_{RH}(b)) = \nu_{RH}(b)/(n-1)!. \tag{25}$$

Proof. See [9]. □

Proposition 8 can be used to compute the weight of some families of graphs, since $w_{RH}(b) = (-1)^{e(b)}\mathrm{Vol}(\mathcal{P}_{RH}(b))$.

4. Ree–Hoover weight of some infinite families of graphs

Here are some of our results concerning new explicit formulas for the Ree–Hoover weight of certain infinite families of graphs. These were first conjectured from numerical values using Ehrhart polynomials. Their proofs use the techniques of *graph homomorphism* and Theorem 4. The weights of 2-connected graphs b are given in absolute value $|w(b)|$, the sign being always equal to $(-1)^{e(b)}$.

Lemma 9. *Suppose that g is a graph over $[n]$ and $i, j \in [n-1]$ are such that g does not contain the edge $\{n, i\}$ but contains the edges $\{i, j\}$ and $\{n, j\}$. In this case, any RH-configuration (h, β) (with $h_n = -1$, $\beta(n) = n$) satisfies one of the following conditions:*

(1) *$h_i = 1$, $h_j = 0$ and $\beta(i) < \beta(j)$,*
(2) *$h_i = -2$, $h_j = -1$ and $\beta(i) > \beta(j)$.*

4.1. **The Ree–Hoover weight of the graph** $K_n\backslash C_k$**.** Let C_k denote the cycle on k elements. For the special case $k = 4$ corresponding to the graph $K_n\backslash C_4$ the proof is different from the one corresponding to the case $k \geq 5$.

Proposition 10 ([9])**.** *For $n \geq 6$, we have*

$$|w_{RH}(K_n\backslash C_4)| = \frac{8}{(n-1)(n-2)(n-3)}, \tag{26}$$

where C_4 is the unoriented cycle with 4 vertices (see Figure 3).

FIGURE 3. The graph C_4

Proposition 11. *For $k \geq 5$, $n \geq k+1$, we have*

$$w_{RH}(K_n\backslash C_k) = 0. \tag{27}$$

Proof. Equation (27) is a consequence of Theorem 4. Indeed, $C_4 \overline{\subseteq} K_n\backslash C_k$, for $k \geq 5$, $n \geq k+1$ and we conclude using (18). □

4.2. **The Ree–Hoover weight of the graph** $K_n\backslash(S_j \cdot C_4 \cdot S_k)$**.** Let $(S_j \cdot C_4 \cdot S_k)$ denote the graph obtained by joining with an edge of the graph C_4 the centres of a j-star and of a k-star. See Figure 4 for an example.

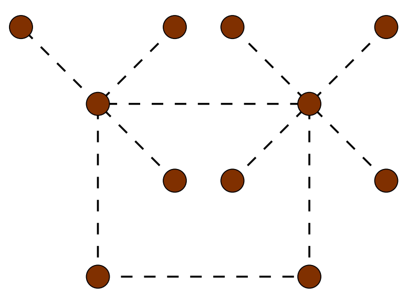

FIGURE 4. The graph $S_3 \cdot C_4 \cdot S_4$

Let us start with the simple case $S_2 \cdot C_4 \cdot S_1$.

Proposition 12. *For $n \geq 8$, we have*

$$|w_{RH}(K_n \backslash (S_2 \cdot C_4 \cdot S_1))| = \frac{4}{(n-1)(n-2)\cdots(n-6)}. \tag{28}$$

Proof. We can assume that the missing edges are $\{1,n\}$, $\{2,n\}$, $\{4,n\}$, $\{1,3\}$, $\{1,5\}$, $\{1,7\}$ and $\{2,3\}$ (see Figure 5).

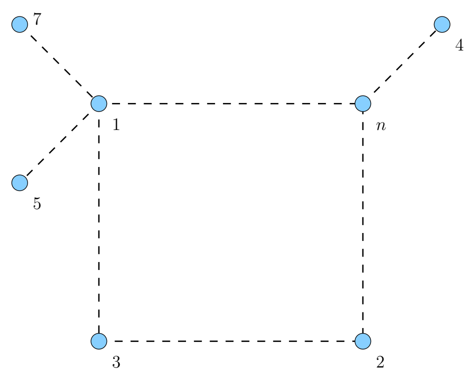

FIGURE 5. The graph $S_2 \cdot C_4 \cdot S_1$

According to Lemma 9 there are two possibilities for h:

- $h_1 = h_2 = h_4 = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(1), \beta(2), \beta(3), \beta(4))$ must be $(6,3,2,1)$ and $(\beta(5), \beta(7))$ must be a permutation of $\{4,5\}$,
- $h_1 = h_2 = h_4 = -2$ and all other $h_i = -1$, so that $(\beta(1), \beta(2), \beta(3), \beta(4))$ must be $(n-6, n-3, n-2, n-1)$ and $(\beta(5), \beta(7))$ must be a permutation of $\{n-4, n-5\}$.

In each case β can be extended in $(n-7)!$ ways, giving the possible relative positions of the $(n-7)$ x_i (see Figure 6). So, there are $2 \cdot 2!\,(n-7)!$ RH-configurations (h, β).

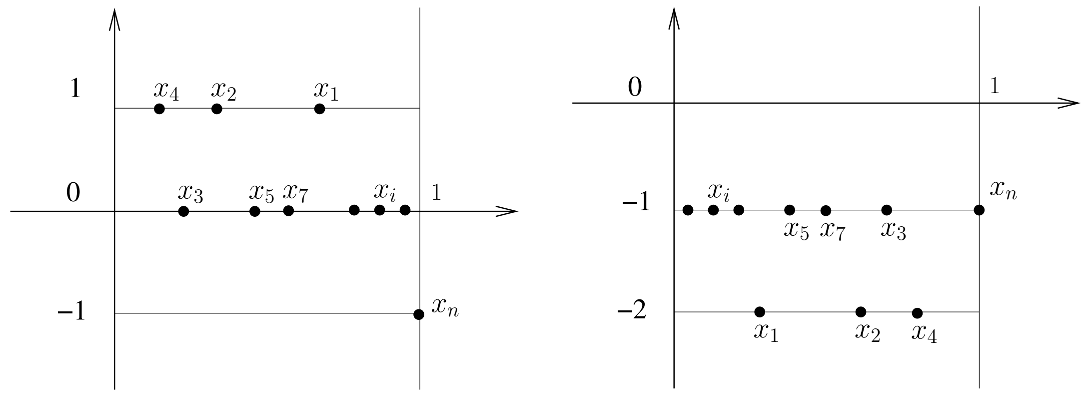

FIGURE 6. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash (S_2 \cdot C_4 \cdot S_1))$

$\square$

In the general case we have the following result.

Proposition 13. *For $j \geq k \geq 1$, $n \geq k + j + 5$, we have*

$$|w_{RH}(K_n \backslash (S_j \cdot C_4 \cdot S_k))| = \frac{2k!\, j!}{(n-1)(n-2)\cdots(n-(k+j+3))}. \tag{29}$$

Proof. We can assume that the missing edges are $\{2, n\}$, $\{4, n\}$, $\{6, n\}$, ..., $\{2k+2, n\}$ and $\{1, 3\}$, $\{1, 5\}$, $\{1, 7\}$, ..., $\{2j + 3, n\}$ and $\{1, n\}$, $\{2, 3\}$ (see Figure 7, for the case of $S_2 \cdot C_4 \cdot S_2$).

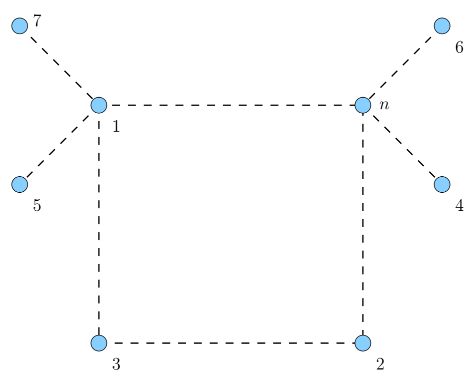

FIGURE 7. The graph $S_2 \cdot C_4 \cdot S_2$

According to Lemma 9 there are two possibilities for h:

- $h_1 = h_2 = h_4 \cdots = h_{2k+2} = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(4), \beta(6), \ldots, \beta(2k+2))$ must be a permutation of $\{1, 2, \ldots, k\}$ and $(\beta(5), \beta(7), \ldots, \beta(2j+3))$ must be a permutation of $\{k+3, k+4, \ldots, k+j+2\}$ and $\beta(3) = k+1$ and $\beta(2) = k+2$ and $\beta(1) = k+j+3$,
- $h_1 = h_2 = h_4 \cdots = h_{2k+2} = -2$ and all other $h_i = -1$, so that $(\beta(4), \beta(6), \ldots, \beta(2k+2))$ must be a permutation of $\{n-1, n-2, \ldots, n-k\}$ and $(\beta(5), \beta(7), \ldots, \beta(2j+3))$ must be a permutation of $\{n-k-3, n-k-4, \ldots, n-k-j-2\}$ and $\beta(3) = n-k-1$ and $\beta(2) = n-k-2$ and $\beta(1) = n-k-j-3$.

In each case β can be extended in $(n-(k+j+4))!$ ways, giving the possible relative positions of the $(n-(k+j+4))$ x_i (see Figure 8, for the case of $S_2 \cdot C_4 \cdot S_2$). So, there are $2 \cdot k!\, j!\, (n-(k+j+4))!$ RH-configurations (h, β).

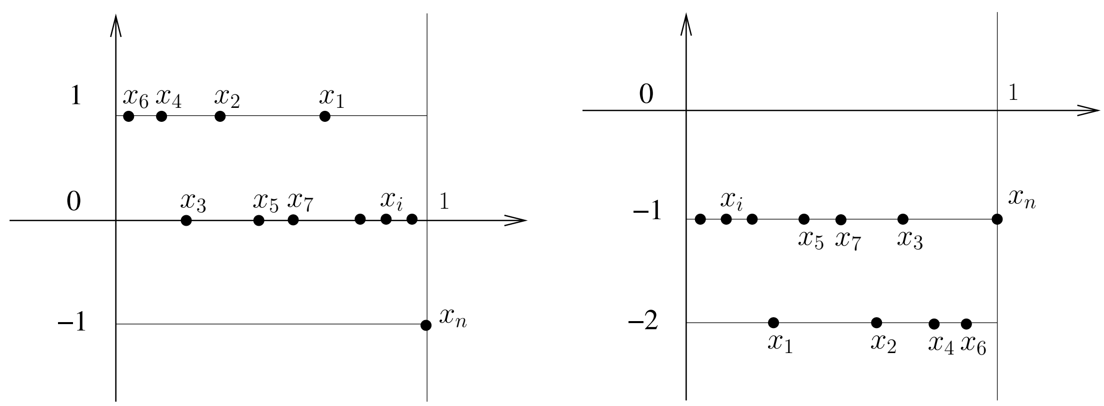

FIGURE 8. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash (S_2 \cdot C_4 \cdot S_2))$

□

4.3. **The Ree–Hoover weight of the graph** $K_n \backslash (S_k \cdot K_3)$**.** Let $S_k \cdot K_3$ denote the graph obtained by identifying one vertex of the graph K_3 with the centre of a k-star. See Figure 9 for an example. $w_{RH}(K_n \backslash (S_k \cdot K_3)) = 0$, for $k \geq 0$, $n \geq k+5$, which is a consequence of Theorem 4. Note that the special case $k = 0$ corresponding to the graph $K_n \backslash K_3$.

4.4. **The Ree–Hoover weight of the graph** $K_n \backslash (S_k \cdot C_p)$**.** Let $S_k \cdot C_p$ denote the graph obtained by identifying one vertex of the graph C_p with the centre of a k-star. See Figure 10 for an example. $w_{RH}(K_n \backslash (S_k \cdot C_p)) = 0$, for $p \geq 5$, $k \geq 1$, $n \geq k+p$, which is a consequence of Theorem 4.

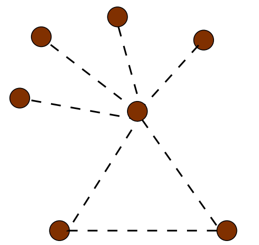

Figure 9. The graph $S_4 \cdot K_3$

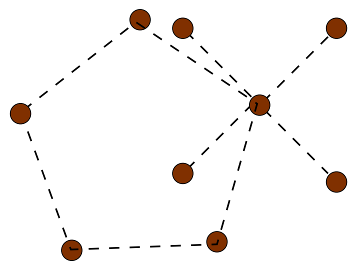

Figure 10. The graph $S_4 \cdot C_5$

4.5. **The Ree–Hoover weight of the graph $K_n \backslash kS_1$.** For $k \geq 2$, $n \geq 2k$, let $K_n \backslash kS_1$ denote the complete graph on n vertices from which k separate edges have been removed, with $S_1 = e$ is the graph with only one edge. See Figure 11 for an example. Then we have $w_{RH}(K_n \backslash kS_1) = w_{RH}(K_n \backslash ke) = 0$, which is a consequence of Theorem 4.

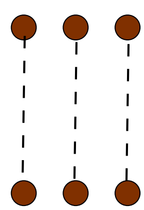

Figure 11. The graph $3S_1$

Note that, for $k = 1$, we have the following result.

Proposition 14 ([9]). *For $n \geq 3$, let $K_n \backslash e$ denote the complete graph on n vertices from which an arbitrary edge has been removed. Then we have*

$$|w_{RH}(K_n \backslash e)| = |w_{RH}(K_n \backslash S_1)| = \frac{2}{(n-1)}. \tag{30}$$

Proof. See [9]. □

Note that the formula (30) is a special case of (31).

4.6. **The Ree–Hoover weight of the graph** $K_n\backslash(S_j \cdot K_3 \cdot S_k)$**.** Let $(S_j \cdot K_3 \cdot S_k)$ denote the graph obtained by joining with an edge of the graph K_3 the centres of a j-star and of a k-star. See Figure 12 for an example. $w_{RH}(K_n\backslash(S_j \cdot K_3 \cdot S_k)) = 0$, for $j \geq k \geq 1$, $n \geq k + j + 4$, which is a consequence of Theorem 4.

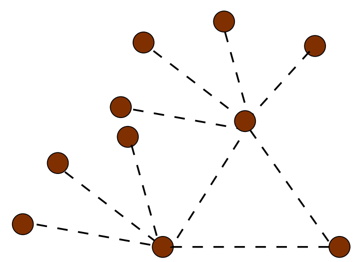

Figure 12. The graph $S_3 \cdot K_3 \cdot S_4$

4.7. **The Ree–Hoover weight of the graph** $K_n\backslash(S_j \cdot C_p \cdot S_k)$**.** Let $(S_j \cdot C_p \cdot S_k)$ denote the graph obtained by joining with an edge of the graph C_p the centres of a j-star and of a k-star. See Figure 13 for an example. $w_{RH}(K_n\backslash(S_j \cdot C_p \cdot S_k)) = 0$, for $p \geq 5$, $j \geq k \geq 1$, $n \geq k + j + p + 1$, which is a consequence of Theorem 4.

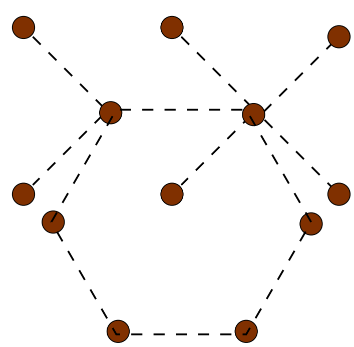

Figure 13. The graph $S_2 \cdot C_6 \cdot S_4$

We need to use Propositions 15–17 to prove Mayer's weight formulas that will be presented in Section 5.

4.8. **The Ree–Hoover weight of the graph $K_n \backslash S_k$.** Let S_k denote the k-star graph with vertex set $[k+1]$ and edge set $\{\{1,2\},\{1,3\},\ldots,\{1,k+1\}\}$, (see Figure 14, for the case of S_3).

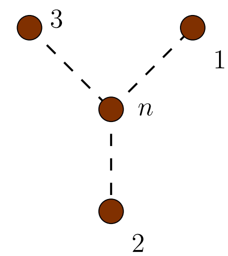

FIGURE 14. The graph S_3

Proposition 15 ([9]). *For $k \geq 1$, $n \geq k+3$, we have*

$$|w_{RH}(K_n \backslash S_k)| = \frac{2k!}{(n-1)(n-2)\cdots(n-k)}. \tag{31}$$

4.9. **The Ree–Hoover weight of the graph $K_n \backslash (S_j – S_k)$.** Let $S_j – S_k$ denote the graph obtained by joining with a new edge the centres of a j-star and of a k-star. See Figure 15 for an example.

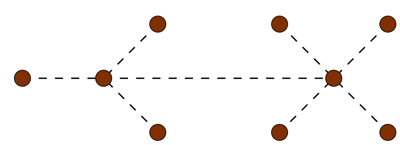

FIGURE 15. The graph $S_3–S_4$

Proposition 16 ([9]). *For $j \geq k \geq 1$, $n \geq k+j+3$, we have*

$$|w_{RH}(K_n \backslash (S_j - S_k))| = \frac{2k!\,j!}{(n-1)(n-2)\cdots(n-(k+j+1))}. \tag{32}$$

4.10. **The Ree–Hoover weight of the graph $K_n \backslash (C_4 \cdot S_k)$.** Let $C_4 \cdot S_k$ denote the graph obtained by identifying one vertex of the graph C_4 with the centre of a k-star. See Figure 16 for an example.

Proposition 17 ([9]). *For $k \geq 1$, $n \geq k+5$, we have*

$$|w_{RH}(K_n \backslash (C_4 \cdot S_k))| = \frac{4k!}{(n-1)(n-2)\cdots(n-(k+3))}. \tag{33}$$

Note that the formula (33) is not a special case of (29).

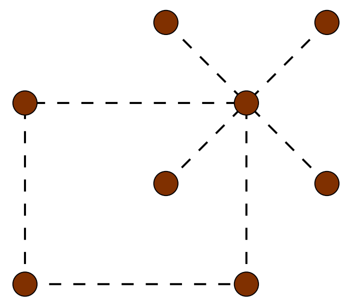

FIGURE 16. The graph $C_4 \cdot S_4$

5. Mayer weight of some infinite families of graphs

In this section, we give explicit formulas for the Mayer weight of the above infinite families of graphs. In order to do so, we use the formula

$$|w_M(b)| = \sum_{b \subseteq d \subseteq K_n} |w_{RH}(d)|, \tag{34}$$

which is a consequence of (11) since $|w_M(b)| = (-1)^{e(b)} w_M(b)$ and $|w_{RH}(d)| = (-1)^{e(d)} w_{RH}(d)$ in the case of hard-core continuum gas in one dimension. Substituting $K_n \backslash g$ and $K_n \backslash k$ for b and d in (34), we have

$$\begin{aligned} |w_M(K_n \backslash g)| &= \sum_{k \subseteq g} |w_{RH}(K_n \backslash k)| \\ &= \sum_{\widetilde{h} \subseteq \widetilde{g}} m(\widetilde{h}, \widetilde{g}) |w_{RH}(K_n \backslash h)|, \end{aligned} \tag{35}$$

where $\widetilde{g}$ denotes the unlabelled graph corresponding to g, $\widetilde{h}$ runs through the unlabelled subgraphs of $\widetilde{g}$, and $m(\widetilde{h}, \widetilde{g})$ is the number of ways of obtaining $\widetilde{h}$ by removing some edges in $\widetilde{h}$. In the following propositions, these multiplicities $m(\widetilde{h}, \widetilde{g})$ are obtainable in each case by direct combinatorial arguments.

5.1. The Mayer weight of the graph $K_n \backslash C_k$.

Proposition 18 ([9]). *For $k = 4$, $n \geq 6$, we have*

$$|w_M(K_n \backslash C_4)| = n + \frac{8}{n-1} + \frac{16}{(n-1)(n-2)} + \frac{16}{(n-1)(n-2)(n-3)}. \tag{36}$$

Proposition 19. *For $n \geq k \geq 5$ we have*

$$|w_M(K_n \backslash C_k)| = n + \frac{2k}{n-1} + \frac{4k}{(n-1)(n-2)} + \frac{2k}{(n-1)(n-2)(n-3)}. \tag{37}$$

Proof. The supergraphs of $K_n\backslash C_k$, $k \geq 5$, whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n\backslash S_1$, $K_n\backslash S_2$, $K_n\backslash(S_1\text{–}S_1)$ and K_n. Their multiplicities are given by the formula

$$|w_M(K_n\backslash C_k)| \;=\; |w_{RH}(K_n)| + \sum_{l=1}^{2} k|w_{RH}(K_n\backslash S_l)| + k|w_{RH}(K_n\backslash(S_1 - S_1))|.$$

We conclude using Propositions 15 and 16. □

Note that the formula (36) is not a special case of (37).

5.2. **The Mayer weight of the graph** $K_n\backslash(S_j \cdot C_4 \cdot S_k)$**.**

Proposition 20. *For $j \geq k \geq 1$, $n \geq k+j+5$, we have, with the usual convention $\binom{k+1}{\ell} = 0$ if $\ell > k+1$,*

$$\begin{aligned}
|w_M(K_n\backslash(S_j \cdot C_4 \cdot S_k))| = n &+ \sum_{l=1}^{j+2} 2\left[\binom{j+2}{l} + \binom{k+2}{l}\right] \frac{l!}{(n-1)\cdots(n-l)} \\
&+ \frac{8}{(n-1)\,(n-2)} + \frac{10}{(n-1)\,(n-2)\,(n-3)} \\
&+ \sum_{l=1}^{j} 4\left[\binom{j}{l} + \binom{k}{l}\right] \frac{l!}{(n-1)\cdots(n-l-3)} \\
&+ \sum_{m=1}^{j}\sum_{l=1}^{k} 2\binom{j}{m}\binom{k}{l} \frac{m!\,l!}{(n-1)\cdots(n-m-l-3)} \\
&+ \sum_{l=1}^{j+1} 2\left[\binom{j+1}{l} + \binom{k+1}{l}\right] \frac{l!}{(n-1)\cdots(n-l-2)} \\
&+ \sum_{m=1}^{j+1}\sum_{l=1}^{k+1} 2\binom{j+1}{m}\binom{k+1}{l} \frac{m!\,l!}{(n-1)\cdots(n-m-l-1)}.
\end{aligned}$$

Proof. The supergraphs of $K_n\backslash(S_j \cdot C_4 \cdot S_k)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n\backslash S_l$, $1 \leq l \leq j+2$, $K_n\backslash(C_4 \cdot S_l)$, $1 \leq l \leq j$, $K_n\backslash(S_m\text{–}S_l)$, $1 \leq m \leq j+1$, $1 \leq l \leq k+1$, $K_n\backslash(S_m \cdot C_4 \cdot S_l)$ $1 \leq m \leq j$, $1 \leq l \leq k$,

C_4 and K_n. Their multiplicities are given by the formula

$$\begin{aligned}|w_M(K_n\backslash(S_j\cdot C_4\cdot S_k))| = |w_{RH}(K_n)| &+ \sum_{l=1}^{j+2}\left[\binom{j+2}{l}+\binom{k+2}{l}\right]|w_{RH}(K_n\backslash S_l)| \\ &+ 2|w_{RH}(K_n\backslash S_2)| + |w_{RH}(K_n\backslash C_4)| + |w_{RH}(K_n\backslash S_1 - S_1)| \\ &+ \sum_{l=1}^{j}\left[\binom{j}{l}+\binom{k}{l}\right]|w_{RH}(K_n\backslash C_4\cdot S_l)| \\ &+ \sum_{m=1}^{j}\sum_{l=1}^{k}\binom{j}{m}\binom{k}{l}|w_{RH}(K_n\backslash S_m\cdot C_4\cdot S_l)| \\ &+ \sum_{l=1}^{j+1}\left[\binom{j+1}{l}+\binom{k+1}{l}\right]|w_{RH}(K_n\backslash(S_1-S_l))| \\ &+ \sum_{m=1}^{j+1}\sum_{l=1}^{k+1}\binom{j+1}{m}\binom{k+1}{l}|w_{RH}(K_n\backslash(S_m-S_l))|.\end{aligned}$$

We conclude using Propositions 10 and 13–17. □

5.3. The Mayer weight of the graph $K_n\backslash(S_k\cdot K_3)$.

Proposition 21. *For $k\geq 0$, $n\geq k+5$, we have*

$$\begin{aligned}|w_M(K_n\backslash(S_k\cdot K_3)| = n &+ \sum_{l=1}^{k+2}2\binom{k+2}{l}\frac{l!}{(n-1)\cdots(n-l)} \\ &+ \sum_{l=1}^{k}4\binom{k}{l}\frac{l!}{(n-1)\cdots(n-l-2)} \\ &+ \frac{2}{(n-1)}+\frac{8}{(n-1)(n-2)}.\end{aligned}$$

Proof. The supergraphs of $K_n\backslash(S_k\cdot K_3)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n\backslash S_l$, $1\leq l\leq k+2$, $K_n\backslash(S_1\text{–}S_l)$, $1\leq l\leq k$ and K_n. Their multiplicities are given by the formula

$$\begin{aligned}|w_M(K_n\backslash(S_k\cdot K_3))| = |w_{RH}(K_n)| &+ \sum_{l=1}^{k+2}\binom{k+2}{l}|w_{RH}(K_n\backslash S_l)| \\ &+ \sum_{l=1}^{k}2\binom{k}{l}|w_{RH}(K_n\backslash(S_1-S_l))| \\ &+ |w_{RH}(K_n\backslash S_1)| + 2|w_{RH}(K_n\backslash S_2)|.\end{aligned}$$

We conclude using Propositions 15 and 16. □

For the special case $k = 0$, $n \geq 5$, we have

$$|w_M(K_n \backslash K_3)| = n + \frac{6}{(n-1)} + \frac{12}{(n-1)(n-2)}. \tag{38}$$

5.4. The Mayer weight of the graph $K_n \backslash (S_k \cdot C_p)$.

Proposition 22. *For $p \geq 5$, $k \geq 1$, $n \geq k + p$, we have*

$$\begin{aligned}|w_M(K_n \backslash (S_k \cdot C_p)| = n &+ \sum_{l=1}^{k+2} 2\binom{k+2}{l} \frac{l!}{(n-1)\cdots(n-l)} \\ &+ \sum_{l=1}^{k+1} 4\left[\binom{k}{l-1} + \binom{k}{l}\right] \frac{l!}{(n-1)\cdots(n-l-2)} \\ &+ \frac{2(p-2)}{(n-1)} + \frac{4(p-1)}{(n-1)(n-2)} + \frac{2p}{(n-1)(n-2)(n-3)}.\end{aligned}$$

Proof. The supergraphs of $K_n \backslash (S_k \cdot C_p)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n \backslash S_l$, $1 \leq l \leq k+2$, $K_n \backslash (S_1 – S_l)$, $1 \leq l \leq k+1$ and K_n. Their multiplicities are given by the formula

$$\begin{aligned}|w_M(K_n \backslash (S_k \cdot C_p))| = |w_{RH}(K_n)| &+ \sum_{l=1}^{k+2} \binom{k+2}{l} |w_{RH}(K_n \backslash S_l)| \\ &+ \sum_{l=1}^{k+1} 2\left[\binom{k}{l-1} + \binom{k}{l}\right] |w_{RH}(K_n \backslash (S_1 - S_l))| \\ &+ (p-2)|w_{RH}(K_n \backslash S_1)| + (p-1)|w_{RH}(K_n \backslash S_2)| \\ &+ p|w_{RH}(K_n \backslash (S_1 - S_1))|.\end{aligned}$$

We conclude using Propositions 15 and 16. □

5.5. The Mayer weight of the graph $K_n \backslash (S_j \cdot K_3 \cdot S_k)$.

Proposition 23. *For $j \geq k \geq 1$, $n \geq k+j+4$, we have, with the usual convention $\binom{k}{\ell} = 0$ if $\ell > k$,*

$$
\begin{aligned}
|w_M(K_n \backslash (S_j \cdot K_3 \cdot S_k))| = n + \sum_{l=1}^{j+2} 2 \left[\binom{j+2}{l} + \binom{k+2}{l} \right] \frac{l!}{(n-1)\cdots(n-l)} \\
- \frac{2}{(n-1)} + \frac{4}{(n-1)\,(n-2)} \\
+ \sum_{l=1}^{j} 4 \left[\binom{j}{l} + \binom{k}{l} \right] \frac{l!}{(n-1)\cdots(n-l-2)} \\
+ \sum_{m=1}^{j+1} \sum_{l=1}^{j} 2 \left[\binom{j}{m}\binom{k}{l} + \binom{j}{m-1}\binom{k}{l} + \binom{j}{l}\binom{k}{m-1} \right] \\
\cdot \frac{m!\,l!}{(n-1)\cdots(n-m-l-1)}.
\end{aligned}
$$

Proof. The supergraphs of $K_n \backslash (S_j \cdot K_3 \cdot S_k)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n \backslash S_l$, $1 \leq l \leq j+2$, $K_n \backslash (S_m – S_l)$, $1 \leq m \leq j+1$, $1 \leq l \leq k+1$ and K_n. Their multiplicities are given by the formula

$$
\begin{aligned}
|w_M(K_n \backslash (S_j \cdot K_3 \cdot S_k))| = |w_{RH}(K_n)| + \sum_{l=1}^{j+2} \left[\binom{j+2}{l} + \binom{k+2}{l} \right] |w_{RH}(K_n \backslash S_l)| \\
- |w_{RH}(K_n \backslash S_1)| + |w_{RH}(K_n \backslash S_2)| \\
+ \sum_{l=1}^{j} 2 \left[\binom{j}{l} + \binom{k}{l} \right] |w_{RH}(K_n \backslash (S_1 - S_l))| \\
+ \sum_{m=1}^{j+1} \sum_{l=1}^{j} \left[\binom{j}{m}\binom{k}{l} + \binom{j}{m-1}\binom{k}{l} + \binom{j}{l}\binom{k}{m-1} \right] \\
\cdot |w_{RH}(K_n \backslash (S_m - S_l))|.
\end{aligned}
$$

We conclude using Propositions 15 and 16. □

5.6. **The Mayer weight of the graph $K_n \backslash (S_j \cdot C_p \cdot S_k)$.**

Proposition 24. *For $p \geq 5$, $j \geq k \geq 1$, $n \geq k+j+p+1$, we have, with the usual convention $\binom{k}{\ell} = 0$ if $\ell > k$,*

$$\begin{aligned}
|w_M(K_n\backslash(S_j \cdot C_p \cdot S_k))| = n &+ \sum_{l=1}^{j+2} 2\left[\binom{j+2}{l} + \binom{k+2}{l}\right] \frac{l!}{(n-1)\cdots(n-l)} \\
&+ \frac{2(p-4)}{(n-1)} + \frac{4(p-2)}{(n-1)\,(n-2)} + \frac{2(p-3)}{(n-1)\,(n-2)\,(n-3)} \\
&+ \sum_{l=1}^{j+1} 2\left[\binom{j+1}{l} + \binom{k+1}{l}\right] \frac{l!}{(n-1)\cdots(n-l-2)} \\
&+ \sum_{m=1}^{j+1}\sum_{l=1}^{k+1} 2\binom{j+1}{m}\binom{k+1}{l} \frac{m!\,l!}{(n-1)\cdots(n-m-l-1)}.
\end{aligned}$$

Proof. The supergraphs of $K_n\backslash(S_j \cdot C_p \cdot S_k)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n\backslash S_l$, $1 \leq l \leq j+2$, $K_n\backslash(S_m\text{–}S_l)$, $1 \leq m \leq j+1$, $1 \leq l \leq k+1$ and K_n. Their multiplicities are given by the formula

$$\begin{aligned}
|w_M(K_n\backslash(S_j \cdot C_p \cdot S_k))| = |w_{RH}(K_n)| &+ \sum_{l=1}^{j+2} \left[\binom{j+2}{l} + \binom{k+2}{l}\right] |w_{RH}(K_n\backslash S_l)| \\
&+ \sum_{l=1}^{j+1} \left[\binom{j+1}{l} + \binom{k+1}{l}\right] |w_{RH}(K_n\backslash(S_1 - S_l))| \\
&+ \sum_{m=1}^{j+1}\sum_{l=1}^{k+1} 2\binom{j+1}{m}\binom{k+1}{l} |w_{RH}(K_n\backslash(S_m - S_l))| \\
&+ (p-4)|w_{RH}(K_n\backslash S_1)| + (p-2)|w_{RH}(K_n\backslash S_2)| \\
&+ (p-3)|w_{RH}(K_n\backslash(S_1 - S_1))|.
\end{aligned}$$

We conclude using Propositions 15 and 16. □

5.7. The Mayer weight of the graph $K_n\backslash kS_1$.

Proposition 25. *For $k \geq 1$, $n \geq 2k$, we have*

$$|w_M(K_n\backslash kS_1)| = n + \frac{2k}{(n-1)}.$$

Proof. The supergraphs of $K_n\backslash kS_1$, $k \geq 1$, whose Ree–Hoover weight is not zero are up to isomorphism of the form $K_n\backslash S_1$ and K_n. Their multiplicities are given by the formula

$$|w_M(K_n\backslash kS_1)| = |w_{RH}(K_n)| + k|w_{RH}(K_n\backslash S_1)|.$$

We conclude using Proposition 15. □

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