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MAYER AND REE–HOOVER WEIGHTS OF INFINITE FAMILIES OF 2-CONNECTED GRAPHS

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Abstract. We study graph weights (i.e., graph invariants) which arise naturally in Mayer's theory and Ree–Hoover's theory of virial expansions in the context of a non-ideal gas. We give special attention to 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. Among our results are explicit formulas for the values of Mayer weights and Ree–Hoover weights for certain infinite families of 2-connected graphs.

Résumé. Nous étudions des poids de graphes (à savoir, des invariants de graphes) qui apparaissent naturellement dans les théories de Mayer et de Ree–Hoover du développement du viriel dans le contexte de gas non-idéaux. Nous nous intéressons spécialement au second poids de Mayer $w_M(c)$ et de Ree–Hoover $w_{RH}(c)$ pour un graphe 2-connexe c provenant d'un gaz à noyaux durs en dimension un. Ces poids sont calculés en utilisant des volumes signés de polytopes convexes associés au graphe c. Parmi nos résultats, nous donnons des formules explicites pour le poids de Mayer et de Ree–Hoover pour certaines familles infinies de graphes 2-connexes.

1. Introduction

Graph weights can be defined as functions on (simple, finite) graphs taking scalar or polynomial values and which are invariant under isomorphism, i.e., under vertex relabelling. Since most graphical concepts share this invariance property, examples of graph weights abound. For instance, the *graph complexity* $\gamma(g)$ of a graph g, which is defined as the number of maximal spanning forests of g, is an example of a graph weight. In the context of a non-ideal gas in a vessel $V \subseteq \mathbb{R}^d$, 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

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

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 real-valued function associated with the pairwise interaction potential of the particles, see [16, 7].

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 [7]):

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

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*). Moreover, 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 $\mathcal{B}[n]$ denote 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 [10] 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 [10, 11, 12] 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).

While physicists are interested in summing the weights of all connected or 2-connected graphs of a given order, the present paper focuses on individual graph contributions and their combinatorial significance. For a given individual graph, the Mayer and Ree–Hoover weights can be computed using Ehrhart polynomials in the case of the hard-core continuum gas in dimension $d = 1$. This has been done systematically for graphs of size ≤ 8 in [5, 6]. The main goal of the present paper is to give exact formulas for certain infinite families of graphs.

In Section 1, we use Möbius inversion to 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 [10, 11]. This rewriting involves special coefficients called star contents. The interest of using the Ree–Hoover weight is that it has the value zero for many graphs. Some general explicit and recursive properties of the star content are given.

Section 2 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. Sufficient conditions for the nullity of the Ree–Hoover weight of a graph are also given. An alternate useful tool, a decomposition of the polytope $\mathcal{P}(c)$ into a certain number of $(n-1)$-dimensional simplices, of volume $1/(n-1)!$ is exploited. This method was introduced in [7] and is called the method of graph homomorphisms. We adapt this method to the context of Ree–Hoover weights. The explicit computation of Mayer or Ree–Hoover weights of particular graphs is very difficult in general and have been made for only certain specific families of graphs (e.g., the complete graphs K_n, the cycle graphs C_n). In the present paper we extend this list to graphs of the form $K_n\backslash g$, where g can be a star graph, a cycle, path graph, or connections of some of these graphs, etc. We give new explicit formulas of the Ree–Hoover weight of these graphs in Section 3. Section 4 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 $e(g)$. If e is an edge of g (i.e. $e \in g$), $g\backslash e$ denotes the graph obtained from g by removing the edge e. If a is a vertex of g, $g\backslash a$ denotes the graph obtained by removing from g vertex a and all its incident edges. 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 $\overline{g} = K_n\backslash g$.

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2. Relations between w_M and w_{RH}

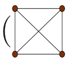
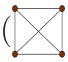
2.1. **Mayer weight, Ree–Hoover weight and star content.** An important rewriting of the virial coefficients was performed by Ree and Hoover [10, 11] by introducing the function

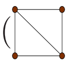
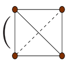
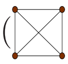
$$\overline{f}(r) = 1 + f(r) \tag{8}$$

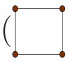
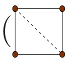
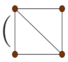
and defining a new weight (denoted here by $w_{RH}(b)$) for 2-connected graphs b, by (9)

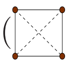
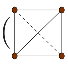
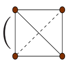
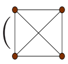
$$w_{RH}(b) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|) \prod_{\{i,j\}\notin b} \overline{f}(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1}\cdots d\overrightarrow{x_{n-1}}, \quad \overrightarrow{x_n} = 0, \tag{9}$$

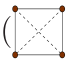
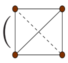
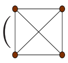
and then expanding each weight $w_M(b)$ by substituting $1 = \overline{f} - f$ for pairs of vertices not connected by edges. Upon performing this rewriting of the Mayer weights series, vertices in the resultant graphs will all be mutually connected by either f bonds (solid lines) or $\overline{f}$ bonds (dotted lines). For example, we have

$w_M($  $) = w_{RH}($  $),$ (10)

$w_M($  $) = w_{RH}($  $) - w_{RH}($  $),$ (11)

$w_M($  $) = w_{MRH}($  $) - w_M($  $)$

$= \{w_{RH}($  $) - w_{RH}($  $)\} - \{w_{RH}($  $) - w_{RH}($  $)\}$

$= w_{RH}($  $) - 2 \cdot w_{RH}($  $) + w_{RH}($  $).$ (12)

In the general situation, using Möbius inversion, it is easy to state formulas linking the two weights w_M and w_{RH}. These formulas are implicit in the work of [11].

Proposition 1. *For a 2-connected graph b, we have*

$$w_{RH}(b) = \sum_{b\subseteq d\subseteq K_n} w_M(d), \tag{13}$$

$$w_M(b) = \sum_{b\subseteq d\subseteq K_n} (-1)^{e(d)-e(b)} w_{RH}(d). \tag{14}$$

Proof. From (9) and the fact that $\overline{f} = 1 + f$, we have

$$\begin{aligned}
w_{RH}(b) &= \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|) \prod_{\{i,j\}\notin b} \overline{f}(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_{n-1}} \\
&= \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|) \prod_{\{i,j\}\in \overline{b}} (1 + f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|))\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_{n-1}} \\
&= \int_{(\mathbb{R}^d)^{n-1}} \sum_{E\subseteq \overline{b}} \prod_{\{i,j\}\in E\cup b} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_{n-1}} \\
&= \int_{(\mathbb{R}^d)^{n-1}} \sum_{b\subseteq d\subseteq K_n} \prod_{\{i,j\}\in d} f(\|\overrightarrow{x_i} - \overrightarrow{x_j}\|)\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_{n-1}} \\
&= \sum_{b\subseteq d\subseteq K_n} w_M(d).
\end{aligned}$$

Using Möbius inversion on (13) for the lattice of subsets of K_n, with the Möbius function $\mu(b, d) = (-1)^{e(d)-e(b)}$, we find (14). □

Remark 1. By the definition of the Ree–Hoover weight, we have in particular

$$w_{RH}(K_n) = w_M(K_n), \quad n \geq 2. \tag{15}$$

When expressing the total weight $|\mathcal{B}[n]|_{w_M}$ in terms of Ree–Hoover weights, there is a new factor which appears for each graph in the expansion of each Mayer weight $w_M(b)$. This factor is called the *star content* by Ree and Hoover [11], and may be either a positive or negative integer.

Definition 2. *Let d be a 2-connected graph over the set $[n] = \{1, 2, \cdots, n\}$. Then, $a_n(d)$, the star content of the graph d, is defined by*

$$a_n(d) = \sum_{\substack{b\subseteq d\\ b\in\mathcal{B}[n]}} (-1)^{e(d)-e(b)}. \tag{16}$$

Proposition 3. *$|\mathcal{B}[n]|_{w_M}$, the total sum of weights of 2-connected graphs over $[n]$ is given by*

$$|\mathcal{B}[n]|_{w_M} = \sum_{d\in\mathcal{B}[n]} a_n(d) w_{RH}(d). \tag{17}$$

Proof. Using (14) we can write $|\mathcal{B}[n]|_{w_M}$ as

$$\begin{aligned}
|\mathcal{B}[n]|_{w_M} &= \sum_{b\in\mathcal{B}[n]} w_M(b) \\
&= \sum_{b\in\mathcal{B}[n]} \sum_{b\subseteq d\subseteq K_n} (-1)^{e(d)-e(b)} w_{RH}(d) \\
&= \sum_{d\in\mathcal{B}[n]} \sum_{\substack{b\subseteq d \\ b\in\mathcal{B}[n]}} (-1)^{e(d)-e(b)} w_{RH}(d) \\
&= \sum_{d\in\mathcal{B}[n]} a_n(d) w_{RH}(d).
\end{aligned}$$

□

So, we can write β_n as

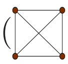
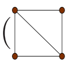
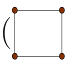
$$\beta_n = \frac{1-n}{n!} \sum_{b\in\mathcal{B}[n]} a_n(b) w_{RH}(b). \tag{18}$$

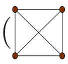
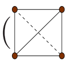
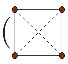
Note that since w_M and w_{RH} are graph invariants, the sum (17) can be simplified as

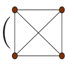
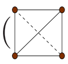
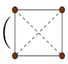
$$\begin{aligned}
|\mathcal{B}[n]|_{w_M} &= \sum_{\widetilde{b}\in\widetilde{\mathcal{B}}[n]} \ell(b) w_M(b) \\
&= \sum_{\widetilde{b}\in\widetilde{\mathcal{B}}[n]} \ell(b) a_n(b) w_{RH}(b),
\end{aligned} \tag{19}$$

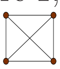
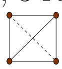
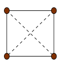
where $\widetilde{\mathcal{B}}[n]$ is the set of unlabelled graphs $\widetilde{b}$ with n vertices and $\ell(b)$ is the number of labellings of $\widetilde{b}$.

For example using the three equations (10)–(12) and (19), the total weight $|\mathcal{B}[4]|_{w_M}$ may be written as

$|\mathcal{B}[4]|_{w_M} = 1 \cdot w_M($$) + 6 \cdot w_M($$) + 3 \cdot w_M($$)$

$= (-2) \cdot w_{RH}($$) + 0 \cdot w_{RH}($$) + 3 \cdot w_{RH}($$)$

$= 1 \cdot (-2) \cdot w_{RH}($$) + 6 \cdot 0 \cdot w_{RH}($$) + 3 \cdot 1 \cdot w_{RH}($$)$, (20)

where 1, 6, 3 represent $\ell(b)$ and (-2), 0, 1 are the star contents $a_4(b)$ of the graphs $b =$ , , , respectively.

Proposition 4. *We have*

$$\sum_{d\in\mathcal{B}[n]} a_n(d) = 1, \tag{21}$$

where $\mathcal{B}[n]$ is the set of all 2*-connected graphs over* $[n]$.

Proof. We have

$$\sum_{d\in\mathcal{B}[n]} a_n(d) = \sum_{d\in\mathcal{B}[n]} \sum_{\substack{b\subseteq d\\ b\in\mathcal{B}[n]}} (-1)^{e(d)-e(b)}$$
$$= \sum_{b\in\mathcal{B}[n]} \sum_{b\subseteq d\subseteq K_n} (-1)^{e(d)-e(b)}.$$

Now, for any two graphs $b, d \in \mathcal{B}[n]$, $b \subseteq d \subseteq K_n$ if and only if $d\backslash b \subseteq K_n\backslash b$. Hence, by the binomial theorem

$$\sum_{b\subseteq d\subseteq K_n} (-1)^{e(d)-e(b)} = \sum_{g\subseteq K_n\backslash b} (-1)^{e(g)}$$
$$= (1+(-1))^{e(K_n\backslash b)}$$

is equal to 1 if $b = K_n$ and 0 otherwise. This concludes the proof of (21). □

2.2. **Star content of some special graphs.** This section is devoted to the study of the star content of some special graphs. We say that a simple graph g over $[n]$ is an *extension* of another graph h over $[n-1]$, if g is obtained from h by adding a new vertex n along with some edges between n and the graph h. Let $g\big|_{[n-1]} = g\backslash n$ denote the restriction of g to the set $[n-1]$ (that is, the vertex n and all its incident edges are removed).

Proposition 5. *Let g a* 2*-connected graph over $[n]$ such that the vertex n is joined to every other vertex and let $g' = g\backslash n$ be the graph obtained from g by removing the vertex n and all its incident edges. Then if g' is also* 2*-connected, we have*

$$a_n(g) = (-1)^{n-1}(n-2)\ a_{n-1}(g'). \tag{22}$$

In order to prove this proposition, we need first the three following lemmas:

Lemma 6. *Let $e = \{a, b\}$ be an edge of a* 2*-connected graph G where the vertex a is a cutpoint of the graph $G\backslash b$. Then, $G\backslash e$ is* 2*-connected.*

Proof. Since G is 2-connected, both a and b are connected to each connected components $C_1, \ldots, C_k$ of $G\backslash a\backslash b$ (see Figure 1). Moreover, since the vertex a is a cutpoint , the number k of components is at least 2. Consider now a vertex c of G. We have to prove $G\backslash c\backslash e$ is connected. Since G is 2-connected, we know that $G\backslash c$ is connected. Now if c is equal to a or b, the graph $G\backslash c\backslash e = G\backslash c$ is connected. If $c \neq a, b$ the vertex c belongs to one of the components $C_1, \ldots, C_k$, say C_1. Moreover a et b are linked by a path of $G\backslash c$ going through C_2. Hence $e = \{a, b\}$ is not an isthmus of $G\backslash c$ and $G\backslash c\backslash e$ is connected. □

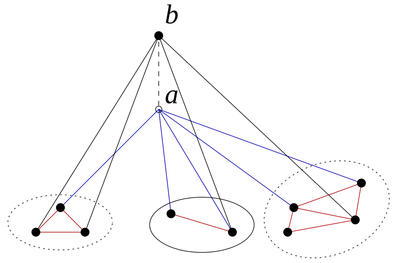


FIGURE 1. A 2-connected graph G with the connected components of $G\backslash b\backslash a$

Lemma 7. *Let h be a 2-connected graph over $[n-1]$. Then we have*

$$\sum_{\substack{g\in\mathcal{B}[n]\\ g\backslash n=h}} (-1)^{e(g)-e(h)} = n-2\cdot \tag{23}$$

Proof. For a 2-connected graph h over the set $[n-1]$, consider the set

$$A = \{g \mid g \text{ is a graph over } [n] \text{ and } g\backslash n = h\},$$

and define a weight function w over A by

$$w(g) = (-1)^{e(g)-e(h)}, \quad \forall g \in A.$$

Consider the following involution Inv_1 acting on the set A:

$$\mathrm{Inv}_1(g) = \begin{cases} g\backslash\{1,n\}, & \text{if } \{1,n\} \in g,\\ g\cup\{1,n\}, & \text{otherwise.}\end{cases}$$

The total weight of the set A, $|A|_w$, is given by

$$|A|_w = \sum_{g\in A}(-1)^{e(g)-e(h)} = |\mathrm{Fix}\ \mathrm{Inv}_1|_w,$$

where Fix Inv_1 denotes the set of all fixed points of the involution Inv_1. It is easy to see that Inv_1 has no fixed point. Hence,

$$|A|_w = \sum_{g\backslash n=h} (-1)^{e(g)-e(h)} = 0. \tag{24}$$

Moreover, there are $n-1$ different ways to obtain an extension g by adding a unique edge between n and h for any 2-connected graph h of size $n-1$. In this case, g is not 2-connected. In the same way, there is only one extension g for h by adding the vertex n without new edge and therefore g is also not connected. If we add the vertex n and two or more edges to the graph h, g is always 2-connected. Then we can write (24) as

$$\begin{aligned} \sum_{\substack{g\in\mathcal{B}[n] \\ g\backslash n=h}} (-1)^{e(g)-e(h)} &= -\sum_{\substack{g\notin\mathcal{B}[n] \\ g\backslash n=h}} (-1)^{e(g)-e(h)} \\ &= -(-(n-1)+1) \\ &= n-2, \end{aligned}$$

which concludes the proof. □

Lemma 8. *Let h be a graph over the set $[n-1]$ which is not 2-connected. Then we have*

$$\sum_{\substack{g\in\mathcal{B}[n] \\ g\backslash n=h}} (-1)^{e(g)} = 0\cdot \tag{25}$$

Proof. For a graph h over the set $[n-1]$ which is not 2-connected, consider the set

$$B = \{g \mid g \text{ is a } 2\text{−connected graph over } [n] \text{ and } g\backslash n = h\}.$$

If h is not connected then $B = \emptyset$ and (25) is trivially satisfied. If h is connected let a be the cutpoint of h having the smallest label. Define the following weight function w over B :

$$w(g) = (-1)^{e(g)}, \quad \forall g \in B.$$

Consider the following involution Inv_2 acting on the set B :

$$\mathrm{Inv}_2(g) = \begin{cases} g\backslash\{a,n\}, & \text{if } \{a,n\} \in g, \\ g \cup \{a,n\}, & \text{otherwise.} \end{cases}$$

Note that for all $g \in B$, $\mathrm{Inv}_2(g)$ is 2-connected by Lemma 6. Hence, B is stable by the involution Inv_2. We deduce that

$$|B|_w = \sum_{g\in B} (-1)^{e(g)} = |\mathrm{Fix}\ \mathrm{Inv}_2|_w,$$

where Fix Inv_2 denotes the set of all fixed points of the involution Inv_2. Again, the involution Inv_2 has no fixed point. Hence,

$$|B|_w = \sum_{g\backslash n=h} (-1)^{e(g)} = 0\cdot$$

□

We are now able to prove Proposition 5.

Proof of Proposition 5. Let g a be 2-connected graph over $[n]$ such that the vertex n is joined to every other vertex and let $g' = g\backslash n$. From (16) we have successively

$$\begin{aligned}
a_n(g) &= \sum_{\substack{h\subseteq g\\ h\in\mathcal{B}[n]}} (-1)^{e(h)-e(g)}\\
&= \sum_{\substack{h\subseteq g\\ h\in\mathcal{B}[n];h\backslash n\in\mathcal{B}[n-1]}} (-1)^{e(h)-e(g)} + \sum_{\substack{h\subseteq g\\ h\in\mathcal{B}[n];h\backslash n\notin\mathcal{B}[n-1]}} (-1)^{e(h)-e(g)}\\
&= \sum_{\substack{h'\subseteq g'\\ h'\in\mathcal{B}[n-1]}} (-1)^{e(g)-e(h')} \sum_{\substack{h\in\mathcal{B}[n]\\ h\backslash n=h'}} (-1)^{e(h)-e(h')}\\
&\qquad\qquad + \sum_{\substack{h'\subseteq g'\\ h'\notin\mathcal{B}[n-1]}} (-1)^{e(g)} \sum_{\substack{h\in\mathcal{B}[n]\\ h\backslash n=h'}} (-1)^{e(h)}\\
&= (-1)^{n-1} \sum_{\substack{h'\subseteq g'\\ h\in\mathcal{B}[n-1]}} (-1)^{e(g')-e(h')}(n-2) + 0 \quad \text{(by Lemmas 7 and 8)}\\
&= (-1)^{n-1}(n-2)a_{n-1}(g')\cdot
\end{aligned}$$

□

Corollary 9. *Let $n > m$ and let g be a 2-connected graph over $[n]$ such that for $i = 0, \ldots, n-m-1$, vertex $n-i$ is joined to every vertex $j < n-i$, and let $g^{(n-m)} = g\backslash n\backslash n-1\backslash\cdots\backslash m+1$ be the graph obtained from g by removing the vertices $n, n-1, \ldots, m+1$ and all their incident edges. Then if $g^{(n-m)}$ is also 2-connected,*

$$a_n(g) = (-1)^{\binom{n}{2}-\binom{m}{2}} \frac{(n-2)!}{(m-2)!}\, a_m(g^{(n-m)}). \tag{26}$$

Remark 2. In particular, taking $g = K_n$ and $m = 2$ in *(26) we have, for $n > 2$,*

$$a_n(K_n) = (-1)^{\binom{n}{2}+1}(n-2)! \tag{27}$$

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

$$w_M(c) = (-1)^{e(c)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\}\in c} \chi(|x_i - x_j| < 1) dx_1 \dots dx_{n-1}, \qquad x_n = 0, \tag{28}$$

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

$$w_{RH}(c) = (-1)^{e(c)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\}\in c} \chi(|x_i - x_j| < 1) \prod_{\{i,j\}\notin c} \chi(|x_i - x_j| > 1) dx_1 \dots dx_{n-1}, \tag{29}$$

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

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

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

$$\begin{aligned}\mathcal{P}_{RH}(c) = \{X \in \mathbb{R}^n \mid x_n = 0, \quad & |x_i - x_j| < 1\, \forall \{i,j\} \in c,\\ & |x_i - x_j| > 1\, \forall \{i,j\} \in \overline{c}\} \subseteq \mathbb{R}^{n-1} \times \{0\} \subseteq \mathbb{R}^n.\end{aligned}$$

3.1. **Why many graphs have Ree–Hoover weight equal to 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 guaranty the nullity of their Ree–Hoover weights. We introduce first some variants of the notion of subgraph and an associated lemma:

Definition 10. *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*

$$g' = g \cap K_{U'}, \tag{30}$$

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 11. *Let g and h be two 2-connected graphs. In the case of hard-core continuum gas in one dimension, we have:*

$$h \mathrel{\overline{\subseteq}} g \quad \text{and} \quad w_{RH}(h) = 0 \quad \text{implies} \quad w_{RH}(g) = 0. \tag{31}$$

Proof. Without loss of generality, we can suppose that h is a subgraph of g where the vertex set of h is $[m]$ and the one of g is $[n]$. By hypothesis, $w_{RH}(h) = 0$, that is, the system S_h of inequalities

$$\begin{aligned} & |x_i - x_j| < 1 \qquad \text{for} \quad \{i,j\} \in h\\ \text{and} \quad & |x_i - x_j| > 1 \qquad \text{for} \quad \{i,j\} \in K_m \backslash h\end{aligned}$$

is contradictory. Consider now the system S_g,

$$\begin{array}{rlll} & |x_i - x_j| < 1 & \text{for} & \{i,j\} \in g \\ \text{and} & |x_i - x_j| > 1 & \text{for} & \{i,j\} \in K_m \backslash g. \end{array}$$

The system S_g has more "<" constraints and more ">" constraints than S_h. Thus, S_g must be also contradictory. That is $w_{RH}(g) = 0$. □

3.2. Sufficient conditions for $w_{RH} = 0$.

Theorem 12. *The Ree–Hoover weight of a 2-connected graph g of size n is zero if g satisfies one of the following conditions,*

$$g \text{ is not chordal } : \exists\, k \geq 4, \quad C_k \,\overline{\subseteq}\, g, \tag{32}$$

$$\text{or } g \text{ has a claw } : S_3 \,\overline{\subseteq}\, g, \tag{33}$$

where S_3 is the 3-star graph (see Figure 4).

Proof.

- In order to prove (32) it is sufficient, by Proposition 11, to show that $w_{RH}(C_k) = 0$, for $k \geq 4$, where C_k is the standard cycle graph $\{\{1,2\},\{2,3\},$ $\ldots,\{k-1,k\},\{1,k\}\}$. Therefore, the associated system of inequalities is contradictory. Without loss of generality, we can assume that $x_1 \leq x_2$. Then $x_2 < x_3$ since $|x_1 - x_2| \leq 1$, $|x_2 - x_3| \leq 1$ and $|x_1 - x_3| \geq 1$. For the same reason $x_i < x_{i+1}$ for all $i = 1,\ldots,k$, with the convention that $x_{k+1} = x_1$. So we obtain $x_1 \leq x_2 < x_3 < \ldots < x_k < x_1$ which is a contradiction.
- In order to prove (33) it is sufficient, by Proposition 11, to show that $w_{RH}(S_3) = 0$ where $S_3 = \{\{1,4\},\{2,4\},\{3,4\}\}$. Without loss of generality, we can assume that $x_4 = 0$, $x_1 \leq x_2 \leq x_3$. Since $|x_i| = |x_i - x_4| < 1$, for $i = 1, 3$, we have $|x_3 - x_1| < 2$. This is incompatible with the conditions $|x_1 - x_2| > 1$, $|x_2 - x_3| > 1$, since $|x_3 - x_1| = (x_3 - x_2) + (x_2 - x_1) > 2$.

□

3.3. The method of graph homomorphisms adapted to the Ree–Hoover weight.

The method of graph homomorphisms was introduced by Labelle, Leroux and Ducharme [7] 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 gases in one dimension. 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 to 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 to the integral parts and the relative positions of the fractional parts of the coordinates $x_1,\ldots,x_n$ of points $X \in \mathcal{P}(b)$.

More precisely, to 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 null or negative. Now consider a 2-connected graph b with vertex set $V = [n] = \{1, 2, \ldots, n\}$, and let $X = (x_1, \ldots, x_n)$ 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, $i = 1, \ldots, n$. 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" $h_1, h_2, \ldots, h_n$ fixed as well as the relative positions (total order) of the fractional parts $\xi_1, \xi_2, \ldots, \xi_n$. Let $h : V \to \mathbb{Z}$ denote 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

$$\mathcal{P}(h,\beta) = \{(h_1 + \xi_1, \ldots, h_{n-1} + \xi_{n-1}, 0) \mid 0 < \xi_{\beta^{-1}(1)} < \cdots < \xi_{\beta^{-1}(n-1)} < 1\} \quad (34)$$

and it is shown in [7] (see also [5] for more details) that each such simplex is affine-equivalent (with jacobian 1) to the standard simplex

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

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

Note that the simplices (34) are disjoint and each such simplex can be characterized by its centre of gravity

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

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 configurations space $\mathbb{R}^{n-1} \times \{0\}$.

Using the fractional coordinates to represent the center of gravity $X_{h,\beta}$ of the simplex $\mathcal{P}(h, \beta)$, and drawing a line segment form $x_i = (h_i, \xi_i)$ 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 and 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 13. ([7]). *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:*

$$\text{for any edge } \{i, j\} \text{ of } b, \quad \beta(i) < \beta(j) \ \text{ implies } \ h_i = h_j \text{ or } h_i = h_j + 1. \tag{35}$$

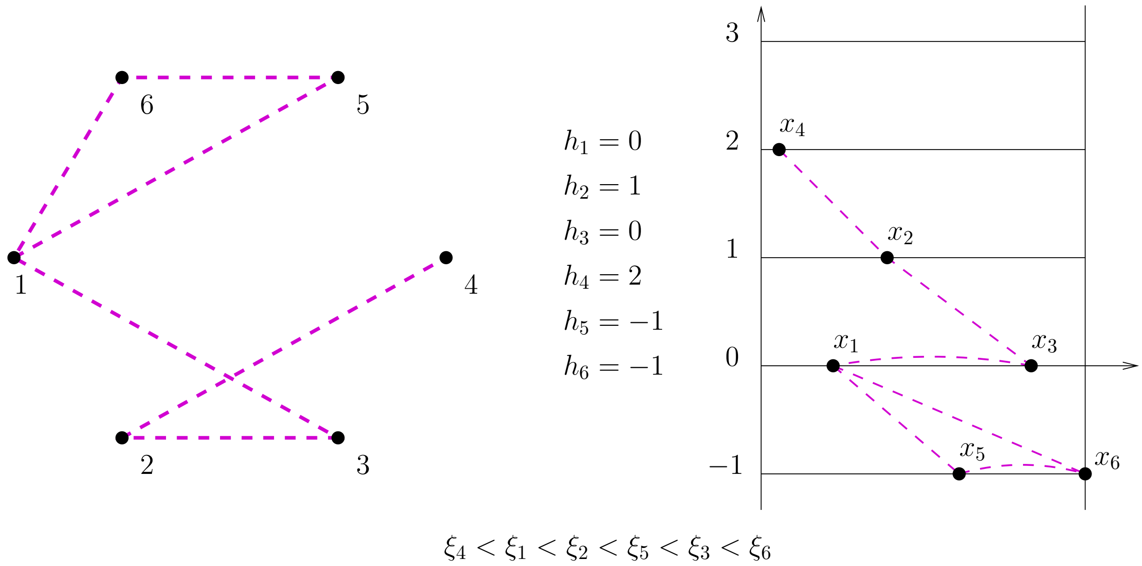


FIGURE 2. Fractional representation of a simplicial subpolytope of a graph b

Corollary 14. ([7]). *Let b be a 2-connected graph and let $\nu(b)$ be the number of pairs (h, β) such that the condition (35) is satisfied. Then the volume of the polytope $\mathcal{P}(b)$ is given by*

$$\mathrm{Vol}(\mathcal{P}(b)) = \nu(b)/(n-1)!. \tag{36}$$

Proposition 14 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 way we can adapt the above configurations to the context of the Ree–Hoover weight.

Proposition 15. *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:*

$$\text{for any edge } \{i,j\} \text{ of } b, \quad \beta(i)<\beta(j) \text{ implies } h_i=h_j \text{ or } h_i=h_j+1, \tag{37}$$

$$\text{for any edge } \{i,j\} \text{ of } \overline{b}, \quad \beta(i)<\beta(j) \text{ implies } h_i\le h_j-1 \text{ or } h_i\ge h_j+2. \tag{38}$$

Proof. Condition (37) expresses exactly that $|x_i-x_j|<1$, whenever $\{i,j\}$ is an edge of b, and condition (38) expresses exactly that $|x_i-x_j|>1$, whenever $\{i,j\}$ is an edge of $\overline{b}$, that is, the defining conditions for the domain of integration of (29). □

Proposition 16. *Let b be a 2-connected graph and let $\nu_{RH}(b)$ be the number of pairs (h,β) such that conditions* (37) *and* (38) *are satisfied. Then the volume of $\mathcal{P}_{RH}(b)$ is given by*

$$\mathrm{Vol}(\mathcal{P}_{RH}(b))=\nu_{RH}(b)/(n-1)!. \tag{39}$$

Proof. It is clear that the polytope $\mathcal{P}_{RH}(b)$ is the disjoint union of all its subpolytopes $\mathcal{P}(h,\beta)$ and the result follows immediately. □

Proposition 16 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 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 homorphisms.* The weights of 2-connected graphs b are given in absolute value $|w(b)|$, the sign being always equal to $(-1)^{e(b)}$.

Lemma 17. *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 either 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 $K_n\backslash S_k$.

Let S_k denote the k-star graph with vertex set $[k+1]$ and edge set $\{\{1,2\},\{1,3\},\ldots,\{1,k+1\}\}$. As a first example, we compute $|w_{RH}(K_n\backslash e)|$, with $K_n\backslash e=K_n\backslash S_1$.

Proposition 18. *For $n\ge 3$, let $K_n\backslash e$ denote the complete graph on n vertices from which an arbitrary edge has been removed. Then we have*

$$|w_{RH}(K_n\backslash e)|=\frac{2}{(n-1)}. \tag{40}$$

Proof. We can assume that the missing edge is $e = \{1, n\}$. According to Lemma 17 with $1, \ldots, k$, $j = k+1, \ldots, n-1$, there are two possibilities for h: a) set $h_1 = 1$, $h_n = -1$ and all other $h_i = 0$, so that $\beta(1)$ must be 1, and b) set $h_1 = -2$ and all other $h_i = -1$, so that $\beta(1)$ must be $n-1$. In both cases β can be extended in $(n-2)!$ ways, giving the possible relative positions of the x_i, $2 \le i \le n-1$ (see Figure 3). So, there are $2(n-2)!$ RH-configurations (h, β).

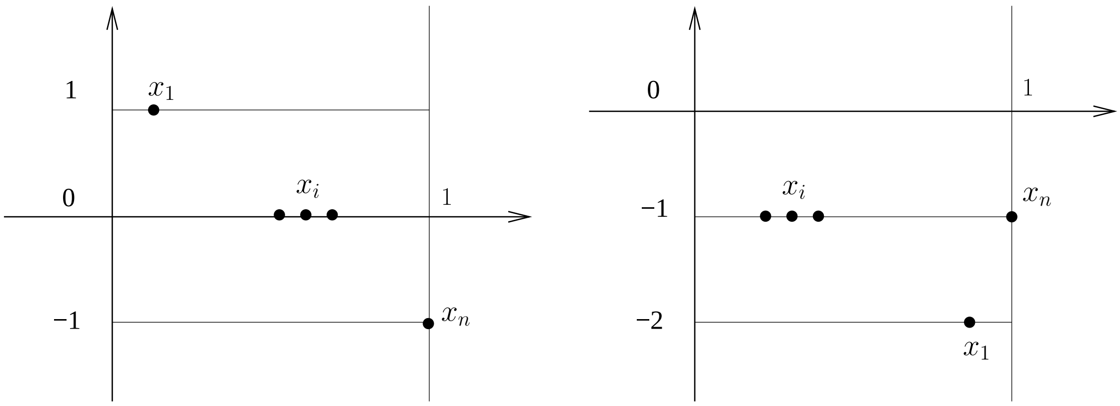


FIGURE 3. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash e)$

□

Note that, from (15) and the known fact that $|w_M(K_n)| = n$, we have

$$w_M(K_n \backslash e) = (-1)^{\binom{n}{2}-1} \left(n + \frac{2}{(n-1)} \right), \tag{41}$$

since

$$|w_M(K_n \backslash e)| = |w_{RH}(K_n)| + |w_{RH}(K_n \backslash e)|.$$

In the general case we have:

Proposition 19. *For $k \ge 1$, $n \ge k+3$, we have*

$$|w_{RH}(K_n \backslash S_k)| = \frac{2k!}{(n-1)(n-2)\cdots(n-k)}. \tag{42}$$

Proof. We assume that the missing edges are $\{1, n\}$, $\{2, n\}$, $\ldots$, $\{k, n\}$ (see Figure 4, for the case of S_3).

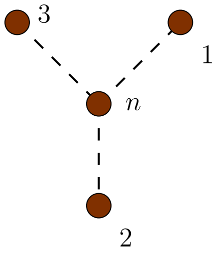


FIGURE 4. The graph S_3

According to Lemma 17 with $1, \ldots, k,\ j = k+1, \ldots, n-1$, there are two possibilities for h:

- $h_1 = h_2 = \cdots = h_k = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(1), \beta(2), \ldots, \beta(k))$ must be a permutation of $\{1, 2, \ldots, k\}$,
- $h_1 = h_2 = \cdots = h_k = -2$ and all other $h_i = -1$, so that $(\beta(1), \beta(2), \ldots, \beta(k))$ must be a permutation of $\{n-1, n-2, \ldots, n-k\}$.

In each case β can be extended in $(n-(k+1))!$ ways, giving the possible relative positions of the x_i, $k+1 \leq i \leq n-1$ (see Figure 5, for the case of S_3). So, there are $2k!(n-k-1)!$ RH-configurations (h, β).

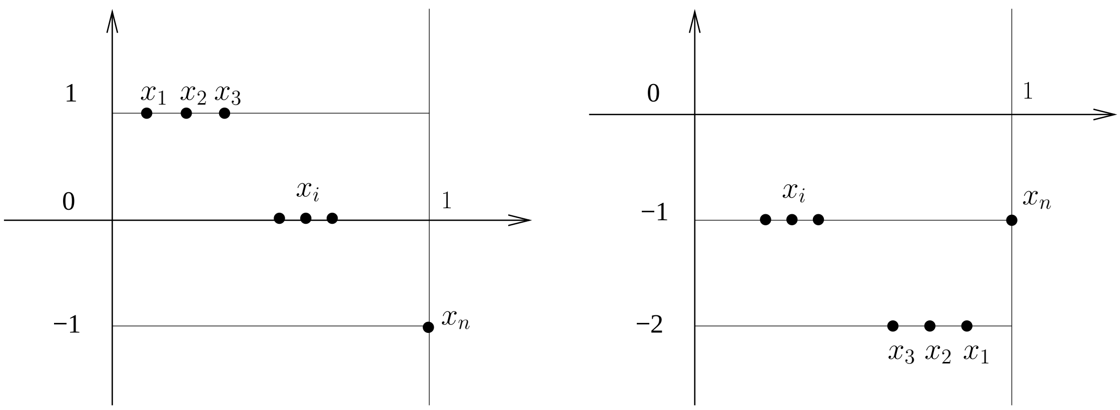


FIGURE 5. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash S_3)$

□

4.2. **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 centers of a j-star and of a k-star. See Figure 6 for an example.

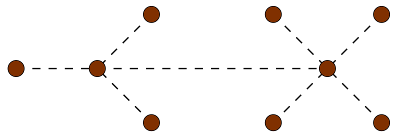


FIGURE 6. The graph S_3–S_4

Let us start with the simple case S_1–S_1.

Proposition 20. *For $n \geq 5$, we have*

$$|w_{RH}(K_n \backslash S_1\text{–}S_1)| = \frac{2}{(n-1)(n-2)(n-3)}. \tag{43}$$

Proof. We can assume that the missing edges are $\{1, n\}$, $\{2, n\}$ and $\{2, 3\}$ (see Figure 7). According to Lemma 17 with $i = 1, \ldots, k+1$ and $j = k+2, \ldots, n-1$ for $i \neq 2$ and $j = k+j+2, \ldots, n-1$ for $i = 2$, there are two possibilities for h:

- $h_1 = h_2 = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(1), \beta(2), \beta(3))$ must be $(1, 3, 2)$,
- $h_1 = h_2 = -2$ and all other $h_i = -1$, so that $(\beta(1), \beta(2), \beta(3))$ must be $(n-1, n-3, n-2)$.

In each case β can be extended in $(n-4)!$ ways, giving the possible relative positions of the x_i, $4 \leq i \leq n-1$ (see Figure 8). So, there are $2(n-4)!$ RH-configurations (h, β).

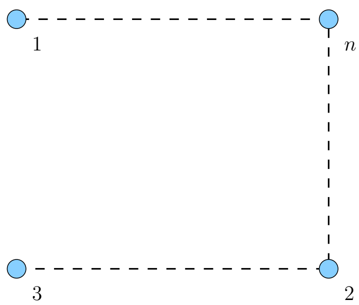


FIGURE 7. The graph S_1–S_1

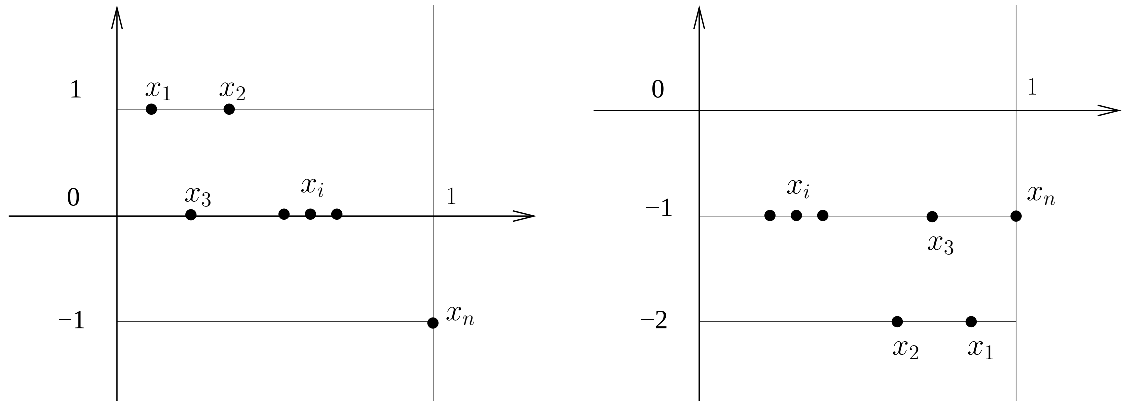


FIGURE 8. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash S_1–S_1)$

□

In the general case we have:

Proposition 21. *For $j \geq k \geq 1$, $n \geq k+j+3$, we have*

$$|w_{RH}(K_n \backslash (S_j–S_k))| = \frac{2k!j!}{(n-1)(n-2)\cdots(n-(k+j+1))}. \quad (44)$$

Proof. We can assume that the missing edges are $\{1,n\}$, $\{2,n\}$, ..., $\{k+1,n\}$ and $\{2,k+2\}$, $\{2,k+3\}$, ...,$\{2,k+j+1\}$ (see Figure 9, for the case of $S_2–S_3$). According to Lemma 17 there are two possibilities for h:

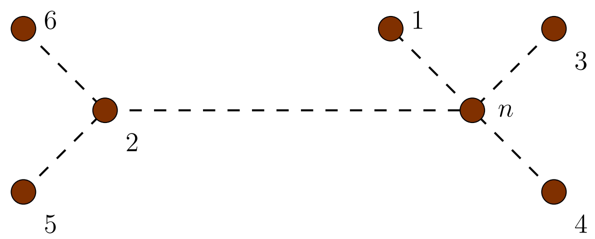


FIGURE 9. The graph $S_2–S_3$

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

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

In each case β can be extended in $(n-(k+j+2))!$ ways, giving the possible relative positions of the x_i, $k+j+2 \leq i \leq n-1$ (see Figure 10, for the case of S_2–S_3). So, there are $2k!j!(n-(k+j+2))!$ RH-configurations (h, β).

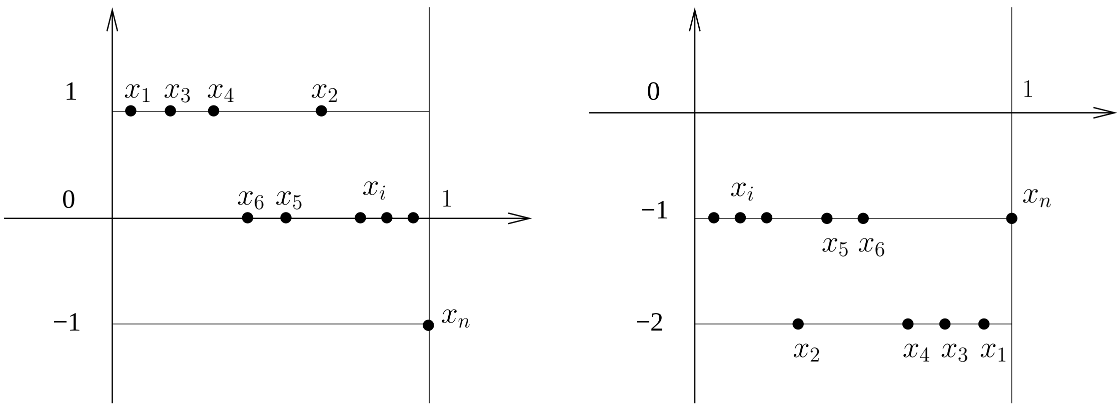


Figure 10. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash S_2\text{–}S_3)$

□

4.3. **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 center of a k-star. See Figure 11 for an example.

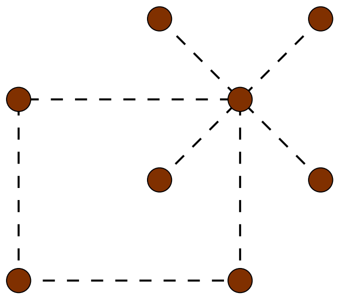


Figure 11. The graph $C_4 \cdot S_4$

Let us start with the special case $k = 0$ corresponding to the graph $K_n \backslash C_4$. The proof is diffferent from the one corresponding to the case $k \geq 1$.

4.3.1. *The Ree–Hoover weight of the graph $K_n \backslash C_4$.*

Proposition 22. *For $n \geq 6$, we have*

$$|w_{RH}(K_n \backslash C_4)| = \frac{8}{(n-1)(n-2)(n-3)}, \tag{45}$$

where C_4 is the unoriented cycle with 4 vertices.

Proof. We can assume that the missing edges are $\{1, n\}$, $\{2, n\}$, $\{2, 3\}$ and $\{3, 1\}$ (see Figure 12). There are four possibilities for h:

- $h_1 = h_2 = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(1), \beta(2))$ must be a permutation of $\{2, 3\}$ and $\beta(3) = 1$,
- $h_1 = h_2 = 1$ and $h_n = h_3 = -1$ and all other $h_i = 0$, so that $(\beta(1), \beta(2))$ must be a permutation of $\{1, 2\}$ and $\beta(3) = n - 1$,
- $h_1 = h_2 = -2$ and all other $h_i = -1$, so that $(\beta(1), \beta(2))$ must be a permutation of $(n-2, n-3)$ and $\beta(3) = n - 1$,
- $h_1 = h_2 = -2$, $h_3 = 0$ and all other $h_i = -1$, so that $(\beta(1), \beta(2))$ must be a permutation of $(n-1, n-2)$ and $\beta(3) = 1$.

In each case β can be extended in $(n-4)!$ ways, giving the possible relative positions of the x_i, $4 \leq i \leq n-1$ (see Figure 13). So, there are $4 \cdot 2!(n-4)!$ RH-configurations (h, β).

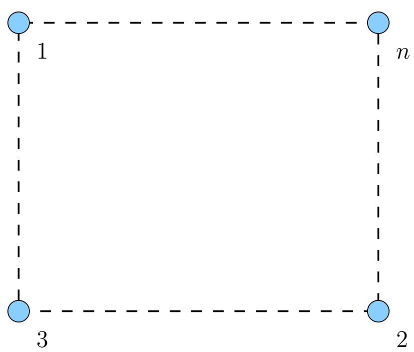


FIGURE 12. The graph C_4

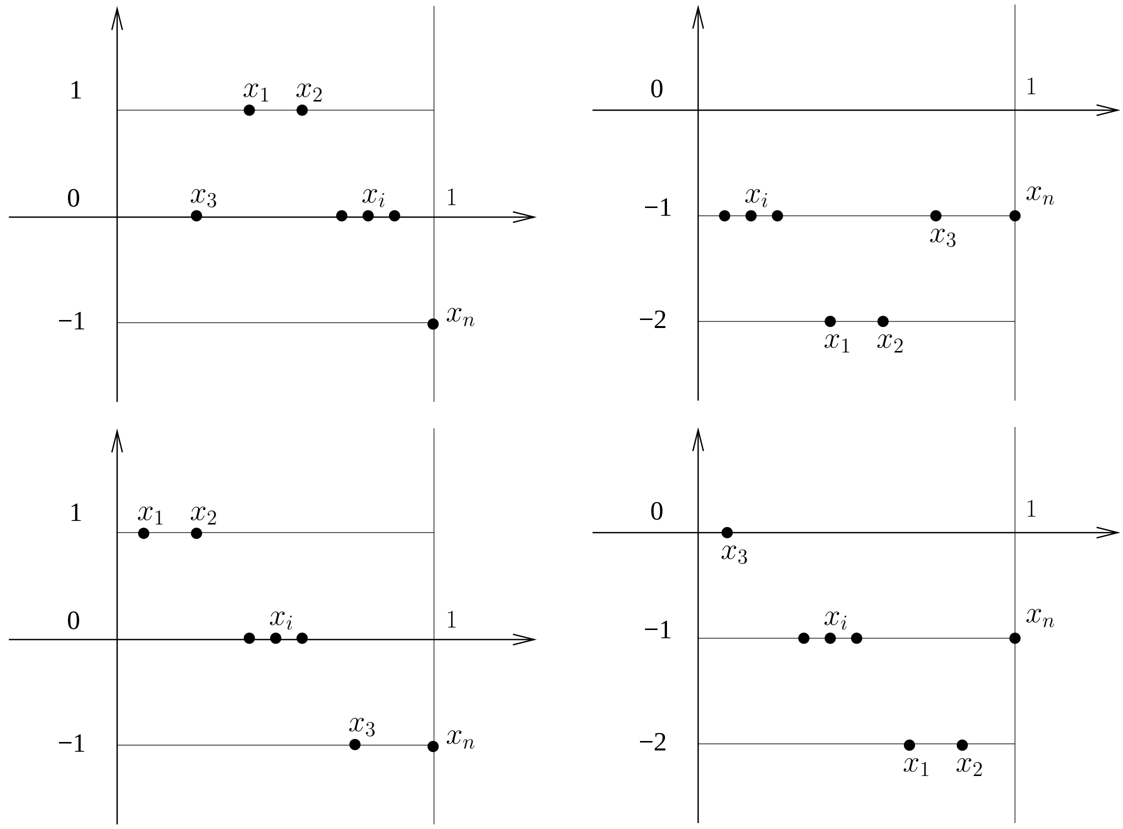


FIGURE 13. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash C_4)$

□

Proposition 23. *For $k \geq 1$, $n \geq k+5$, we have*

$$|w_{RH}(K_n \backslash (C_4 \cdot S_k))| = \frac{4k!}{(n-1)(n-2)\cdots(n-(k+3))}. \tag{46}$$

Proof. We can assume that the missing edges are $\{1, n\}$, $\{2, n\}$, $\{4, n\}$, $\ldots$, $\{k+3, n\}$ and $\{1, 3\}$, $\{2, 3\}$ (see Figure 14, for the case of $C_4 \cdot S_2$).

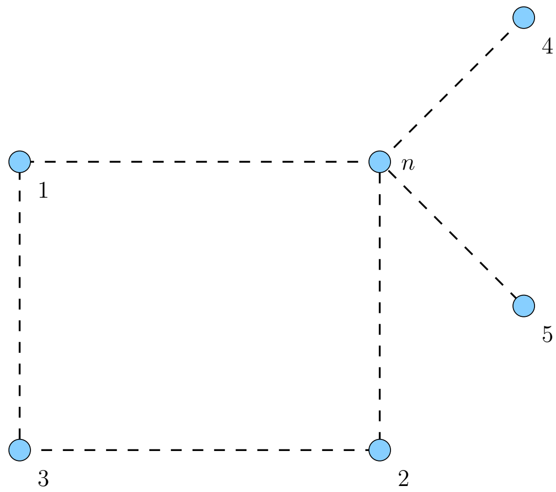


FIGURE 14. The graph $C_4 \cdot S_2$

According to Lemma 17 there are two possibilities for h:

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

In each case β can be extended in $(n-(k+4))!$ ways, giving the possible relative positions of the x_i, $k+4 \leq i \leq n-1$ (see Figure 15, for the case of $C_4 \cdot S_2$). So, there are $2 \cdot 2!\, k!\, (n-(k+4))!$ RH-configurations (h, β).

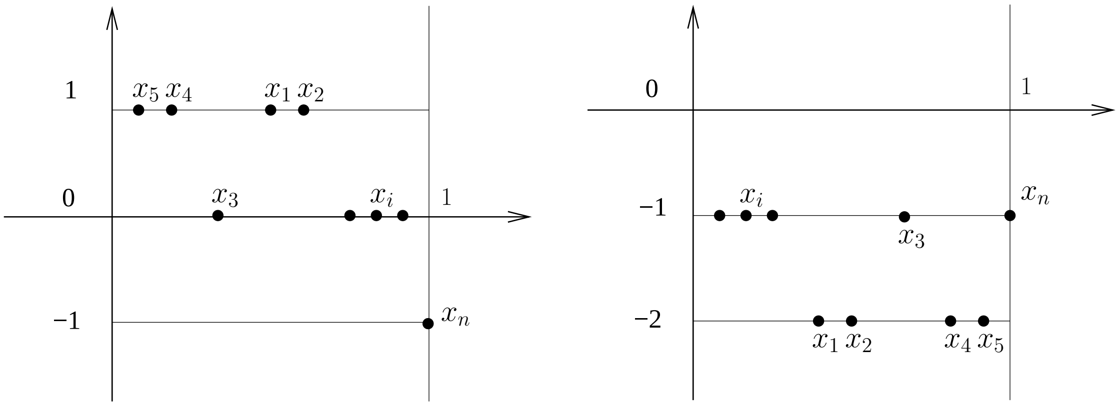


FIGURE 15. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}(K_n \backslash (C_4 \cdot S_2))$

□

Note that the formula (45) is not a special case of (46).

4.4. **The Ree–Hoover weight of the graph** $K_n \backslash P_k$**.** Let P_k denote the path graph with vertex set $[k]$ and edge set $\{\{1,2\},\{2,3\},\ldots,\{k-1,k\}\}$. For $n \geq 5$, we have $K_n \backslash P_3 = K_n \backslash S_2$ and $K_n \backslash P_4 = K_n \backslash S_1$–$S_1$. Thus, the weights $w_{RH}(K_n \backslash P_3)$ and $w_{RH}(K_n \backslash P_4)$ can be obtained as special cases of Propositions 19 and 20. Moreover, $w_{RH}(K_n \backslash P_k) = 0$, for $k \geq 5$, $n \geq k+1$, which is a consequence of Theorem 12. Indeed, $C_4 \mathrel{\overline{\subseteq}} K_n \backslash P_k$ and we conclude using (32).

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 following formula

$$|w_M(b)| = \sum_{b \subseteq d \subseteq K_n} |w_{RH}(d)| \qquad (47)$$

which is a consequence of (14) 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 gases in one dimension. Substituting $K_n \backslash g$ and $K_n \backslash k$ for b and d in (47), we have

$$\begin{aligned} |w_M(K_n \backslash g)| &= \sum_{k \subseteq g} |w_{RH}(K_n \backslash k)| \\ &= \sum_{\widetilde{h} \subseteq \widetilde{g}} m(\widetilde{h}, \widetilde{g}) |w_{RH}(K_n \backslash h)|, \qquad (48) \end{aligned}$$

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 $K_n\backslash S_k$.**

Proposition 24. *For $k \geq 1$, $n \geq k+3$, we have*

$$|w_M(K_n\backslash S_k)| = n + 2\sum_{j=1}^{k} \frac{j!\binom{k}{j}}{(n-1)(n-2)\cdots(n-j)}.$$

Proof. The over graphs of $K_n\backslash S_k$ are up to isomorphism of the form: $K_n\backslash S_j$, $1 \leq j \leq k$ and K_n. Their multiplicities $m(S_j, S_k)$ are given by $m(S_j, S_k) = \binom{k}{j}$ because one has to choose j edges among the k edges incident to the center of the star. Note that $S_0 = \emptyset$ is the star with no edge. Hence,

$$|w_M(K_n\backslash S_k)| = \sum_{j=0}^{k} \binom{k}{j} |w_{RH}(K_n\backslash S_j)|.$$

We conclude using Proposition 19. □

5.2. **The Mayer weight of the graph $K_n\backslash S_j$–S_k.**

Proposition 25. *For $j \geq k \geq 1$, $n \geq k+j+3$, we have, with the usual convention $\binom{k+1}{\ell} = 0$ if $\ell > k+1$,*

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

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

$$m(S_l, S_j\text{–}S_k) = \tbinom{j+1}{l} + \tbinom{k+1}{l},\ l \geq 2, \quad m(S_1, S_j\text{–}S_k) = \tbinom{j+1}{l} + \tbinom{k+1}{l} - 1,$$
$$m(S_m\text{–}S_l, S_j\text{–}S_k) = \tbinom{j}{m}\tbinom{k}{l}.$$

Hence,

$$|w_M(K_n\backslash(S_j\text{–}S_k))| = |w_{RH}(K_n)| + \sum_{l=1}^{j+1}\left[\binom{j+1}{l} + \binom{k+1}{l}\right]|w_{RH}(K_n\backslash S_l)| + \sum_{m=1}^{j}\sum_{l=1}^{k}\binom{j}{m}\binom{k}{l}|w_{RH}(K_n\backslash(S_m\text{–}S_l))| - |w_{RH}(K_n\backslash S_1)|.$$

We conclude using Propositions 19 and 21. □

5.3. **The Mayer weight of the graph $K_n\backslash C_4$.**

Proposition 26. *For $n \geq 6$, we have*

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

Proof. Note first that the RH-weight of the over graph $K_n\backslash S_1\backslash S_1$ of $K_n\backslash C_4$ is 0. The other over graphs of $K_n\backslash C_4$ are, up to isomorphism, of the form: $K_n\backslash S_1$, $K_n\backslash S_2$, $K_n\backslash C_4$, $K_n\backslash(S_1 - S_1)$ and K_n. Their multiplicities are given by

$$m(S_l, C_4) = 4,\ 1 \leq l \leq 2, \quad m(S_1\text{–}S_1, C_4) = 4.$$

Hence,

$$|w_M(K_n\backslash C_4)| = |w_{RH}(K_n)| + \sum_{l=1}^{2} 4|w_{RH}(K_n\backslash S_l)| + 4|w_{RH}(K_n\backslash(S_1 - S_1))| + |w_{RH}(K_n\backslash C_4)|.$$

We conclude using Propositions 19, 20 and 22. □

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

Proposition 27. *For $k \geq 1$, $n \geq k+5$, we have*

$$\begin{aligned}|w_M(K_n\backslash(C_4 \cdot S_k))| = n &+ \sum_{l=1}^{k+2} 2\binom{k+2}{l}\frac{l!}{(n-1)\cdots(n-l)} \\ &+ \sum_{l=1}^{k} 4\binom{k}{l}\frac{l!}{(n-1)\cdots(n-(l+3))} \\ &+ \sum_{l=1}^{k+1} 4\left[\binom{k}{l-1} + \binom{k}{l}\right]\frac{l!}{(n-1)\cdots(n-(l+2))} \\ &+ \frac{4}{n-1} + \frac{12}{(n-1)\,(n-2)} + \frac{16}{(n-1)\,(n-2)\,(n-3)}.\end{aligned}$$

Proof. The over graphs of $K_n\backslash(C_4\cdot S_k)$ whose Ree–Hoover weight is not zero are up to isomorphism of the form: $K_n\backslash S_l$, $1\le l\le k+2$, $K_n\backslash(C_4\cdot S_l)$, $1\le l\le k$, $K_n\backslash(S_1\text{–}S_l)$, $1\le l\le k+1$, C_4 and K_n. Their multiplicities are given by

$$\begin{aligned}&m(S_l,C_4\cdot S_k)=\tbinom{k+2}{l},\ l\ge 3,\quad m(S_1,C_4\cdot S_k)=\tbinom{k+2}{l}+2,\\&m(S_2,C_4\cdot S_k)=\tbinom{k+2}{l}+3,\quad m(C_4\cdot S_l,C_4\cdot S_k)=\tbinom{k}{l},\\&m(S_1\text{–}S_l,C_4\cdot S_k)=2\left[\tbinom{k}{l-1}+\tbinom{k}{l}\right],\ l\ge 2,\quad m(S_1\text{–}S_1,C_4\cdot S_k)=2\tbinom{k}{1}+4.\end{aligned}$$

Hence,

$$\begin{aligned}|w_M(C_4\cdot S_k)|=|w_{RH}(K_n)|&+\sum_{l=1}^{k+2}\binom{k+2}{l}|w_{RH}(K_n\backslash S_l)|\\&+\sum_{l=1}^{k}\binom{k}{l}|w_{RH}(K_n\backslash C_4\cdot S_l)|+2|w_{RH}(K_n\backslash S_1)|\\&+\sum_{l=1}^{k+1}2\left[\binom{k}{l-1}+\binom{k}{l}\right]|w_{RH}(K_n\backslash(S_1-S_l))|\\&+3|w_{RH}(K_n\backslash S_2)|+|w_{RH}(K_n\backslash C_4)|+4|w_{RH}(K_n\backslash S_1-S_1)|.\end{aligned}$$

We conclude using Propositions 19–23. □

5.5. The Mayer weight of the graph $K_n\backslash P_k$.

Proposition 28. *For $k\ge 5$, $n\ge k+1$, we have*

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

Proof. The over graphs of $K_n\backslash P_k$, $k\ge 5$, whose Ree–Hoover weight is not zero are up to isomorphism of the form: $K_n\backslash S_1$, $K_n\backslash S_2$, $K_n\backslash P_4$ and K_n. Their multiplicities are given by

$$m(S_l,P_k)=k-l,\ 1\le l\le 2,\quad m(P_4,P_k)=k-3.$$

Hence,

$$\begin{aligned}|w_M(K_n\backslash P_k)|=|w_{RH}(K_n)|&+(k-1)|w_{RH}(K_n\backslash S_1)|\\&+(k-2)|w_{RH}(K_n\backslash S_2)|+(k-3)|w_{RH}(K_n\backslash P_4)|.\end{aligned}$$

We conclude using Propositions 19 and 20. □

References

[1] O. Bernardi, "Solution to a combinatorial puzzle arising from Mayer's theory of cluster integrals." *Séminaire Lotharingien de Combinatoire* **59** (2008), Article B59e.

[2] N. Clisby and B. M. McCoy, "Negative virial coefficients and the dominance of loose packed diagrams for D-dimensional hard spheres." *Journal of Statistical Physics* **114** (2004), 1361–1392.

[3] N. Clisby and B. M. McCoy, "Ninth and tenth order virial coefficients for hard spheres in D dimensions." *Journal of Statistical Physics* **122** (2006), 15–57.

[4] N. Clisby, *Negative Virial Coefficients for Hard Spheres.* PhD thesis, Stony Brook University, Stony Brook, New York, May (2004).

[5] A. Kaouche, *Invariants de graphes liés aux gaz imparfaits.* PhD thesis, Université du Québec à Montréal, 2009.

[6] A. Kaouche and P. Leroux, "Tables for the Mayer and Ree–Hoover graph weights of 2-connected graphs of size 4 to 7." [`http://www.lacim.uqam.ca/~kaouche/TableauRH7.pdf`] "Tables for the Mayer and Ree–Hoover graph weights of 2-connected graphs of size 8." [`http://www.lacim.uqam.ca/~kaouche/TableauRH8.pdf`] (2007).

[7] G. Labelle, P. Leroux and M. G. Ducharme, "Graph weights arising from Mayer's theory of cluster integrals." *Séminaire Lotharingien de Combinatoire* **54** (2007), Article B54m.

[8] P. Leroux, "Enumerative problems inspired by Mayer's theory of cluster integrals." *The Electronic Journal of Combinatorics* **11**(1) (2004), Article R32.

[9] J. E. Mayer and M. G. Mayer, *Statistical Mechanics.* New York: Wiley (1940).

[10] F. H. Ree and W. G. Hoover, "Fifth and sixth virial coefficients for hard spheres and hard discs." *The Journal of Chemical Physics* **40** (1964), 939–950.

[11] F. H. Ree and W. G. Hoover, "Reformulation of the virial series for classical fluids." *The Journal of Chemical Physics* **41** (1964), 1635–1645.

[12] F. H. Ree and W. G. Hoover, "Seventh virial coefficients for hard spheres and hard discs." *The Journal of Chemical Physics* **46** (1967), 4181–4196.

[13] R. J. Riddell and G. E. Uhlenbeck, "On the Theory of the virial development of the equation of state of monoatomic gases." *The Journal of Chemical Physics* **21** (1953), 2056–2064.

[14] D. Ruelle, *Statistical mechanics*, Addison-Wesley (1989).

[15] R. P. Stanley, *Enumerative Combinatorics,* vol. 1, Belmont, California: Wadsworth (1986).

[16] G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics,* Providence, Rhode Island: American Mathematical Society (1963), 181 pp.

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