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Other Formulas for the Ree-Hoover and Mayer Weights of Families of 2-Connected Graphs

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Abstract

We study graph weights which naturally occur in Mayer's theory and Ree-Hoover's theory for the virial expansion in the context of an imperfect gas. We pay particular attention to the Mayer weight and Ree-Hoover weight of a 2-connected graph in the case of the hard-core continuum gas in one dimension. These weights are calculated from signed volumes of convex polytopes associated with the graph. In the present paper, we use the method of graph homomorphisms, to develop other explicit formulas of Mayer weights and Ree-Hoover weights for infinite families of 2-connected graphs.

Keywords

Combinatorial, Mayer Weight, Statistical Mechanics, Ree-Hoover Weight, Graph Invariants, Virial Expansion

1. Introduction

Before discussing our subject, we first present some preliminary notions on the theory of graphs drawn from among others [1] [2] [3].

Preliminary Notions on the Theory of Graphs

Definition 1. *A* simple graph g *is formed of two sets: a non-empty finite set* V*, called the set of vertices of* g*, and a set* E *of pairs of vertices, called the set of edges of* g*. So we have* $E \subseteq \mathcal{P}_2(V)$ *with* $\mathcal{P}_2(V)$ *denotes all the parts of* V *with two elements. We often write* $g = (V, E)$.

Definition 2. *A* subgraph h *of a graph* $g = (V, E)$ *is a graph of the form* $h = (V_0, E_0)$*, such that* $V_0 \subseteq V$ *and* $E_0 = \mathcal{P}_2(V_0) \cap E$.

Definition 3. *An* over graph g *of a graph* $h = (V, E)$ *is a graph of the form* $g = (V_1, E_1)$*, such that* $V \subseteq V_1$ *and* $E = \mathcal{P}_2(V) \cap E_1$.

In the present work it will be useful to identify a graph with all of its edges, that is to say $g \subseteq \mathcal{P}_2(V)$.

Definition 4. *In a simple graph* $g = (V, E)$, *a* chain c *is a finite sequence of vertices,* $v_0, v_1, \cdots, v_m$, *such that for all* $0 \le i < m$, $\{v_i, v_{i+1}\} \in E$. *We write* $c = [v_0, v_1, \cdots, v_m]$.

Definition 5. *A graph* $g = (V, E)$ *is* connected *if* $\forall v, w \in V$, *there is a chain from v to w.*

Any graph breaks down uniquely as a disjoint union of connected graphs.

Definition 6. *On the set V of the vertices of the simple graph* $g = (V, E)$, *we define the relation of equivalence:* $v \sim w \iff$ *there is a chain v to w in g. Let* $V_1, V_2, \cdots, V_k$ *the equivalence classes of* $\sim$ *and let's say, for* $1 \le i \le k$, $g_i = g_{V_i}$, *the subgraph of g generated by* V_i. *These simple graphs* g_i, *that we call the* connected components *of g, are related* (see Figure 1 *with connected components are circled*).

Definition 7. *A* cutpoint (or articulation point) *of a connected graph c is a vertex of c whose removal yields a disconnected graph.*

Definition 8. *A connected graph is called* 2*-connected if it has no cutpoint* (see Figure 2).

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 $[n] = \{1, 2, \cdots, n\}$ of vertices, is defined by (see [1] [4] [5] [6])

$$w_M(c) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\} \in c} f\left(\left\|\mathbf{x}_i - \mathbf{x}_j\right\|\right) \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_{n-1}, \quad \mathbf{x}_n = 0, \tag{1}$$

where $\mathbf{x}_1, \cdots, \mathbf{x}_n$ are variables in $\mathbb{R}^d$ representing the positions of n particles in V ($V \to \infty$), the value $\mathbf{x}_n = 0$ being arbitrarily fixed, and where $f = f(r)$ is a real-valued function associated with the pairwise interaction potential of the particles, see [6] [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

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

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 [6]):

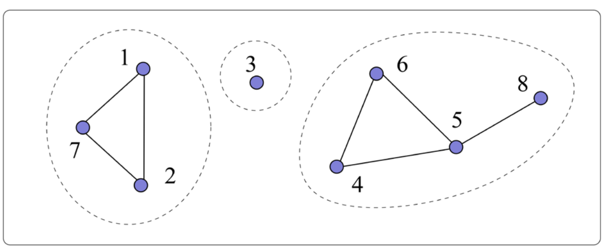

Figure 1. A simple graph and its connected components.

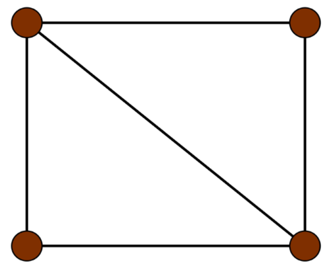

Figure 2. A 2-connected graph.

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

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*). The Mayer weight appear 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

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

where $\mathcal{B}[n]$ denote the set of 2-connected graphs over $[n]$ and $\left|\mathcal{B}[n]\right|_{w_M}$ is the total sum of weights of 2-connected graphs over $[n]$. In order to compute this expansion numerically, Ree and Hoover [8] introduced a modified weight denoted by $w_{RH}(b)$, for 2-connected graphs b, which greatly simplifies the computations. It is defined by

$$w_{RH}(b) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in b} f\left(\left\|\boldsymbol{x}_i - \boldsymbol{x}_j\right\|\right) \prod_{\{i,j\}\notin b} \overline{f}\left(\left\|\boldsymbol{x}_i - \boldsymbol{x}_j\right\|\right) \mathrm{d}\boldsymbol{x}_1 \cdots \mathrm{d}\boldsymbol{x}_{n-1}, \quad \boldsymbol{x}_n = 0, \tag{6}$$

where $\overline{f}(r) = 1 + f(r)$. Using this new weight, Ree and Hoover [8] [9] [10] and later Clisby and McCoy [11] [12] [13] 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 denote 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 [1] [14].

In Section 2, we look at the 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 utilised. This method was introduced in [6] and was adapted in [1] [5] 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 challenging in general and have been made for only certain specific families of graphs (see [4] [5] [6] [15] [16] [17] [18]). In the present paper we extend this list to include other graphs. 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.* $e\in g$), $g\setminus e$ denotes 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 $[n]=\{1,2,\cdots,n\}$ is denoted by K_n. The complementary graph of a subgraph $g\subseteq K_n$ is the graph $\overline{g}=K_n\setminus g$.

An important rewriting of the virial coefficients was performed by Ree and Hoover [8] [9] 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)

$$w_{RH}(b)=\int_{(\mathbb{R}^d)^{n-1}}\prod_{\{i,j\}\in b}f(\|\boldsymbol{x}_i-\boldsymbol{x}_j\|)\prod_{\{i,j\}\notin b}\overline{f}(\|\boldsymbol{x}_i-\boldsymbol{x}_j\|)\mathrm{d}\boldsymbol{x}_1\cdots\mathrm{d}\boldsymbol{x}_{n-1},\ \ \boldsymbol{x}_n=0, \tag{9}$$

and then expanding each weight $w_M(b)$ by substituting $1=\overline{f}-f$ for pairs of vertices not connected by edges.

In [1], we gived explicit linear relations expressing the Ree-Hoover weights in terms of the Mayer weights and vice versa: For a 2-connected graph *b*, we have

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

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

So that 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 (1.12) 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

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

2. 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

$$w_M(c)=(-1)^{e(c)}\int_{\mathbb{R}^{n-1}}\prod_{\{i,j\}\in c}\chi\left(\left|x_i-x_j\right|<1\right)\mathrm{d}x_1\cdots\mathrm{d}x_{n-1},\ x_n=0, \tag{14}$$

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

$$w_{RH}(c)=(-1)^{e(c)}\int_{\mathbb{R}^{n-1}}\prod_{\{i,j\}\in c}\chi\left(\left|x_i-x_j\right|<1\right)\prod_{\{i,j\}\notin c}\chi\left(\left|x_i-x_j\right|>1\right)\mathrm{d}x_1\cdots\mathrm{d}x_{n-1}, \tag{15}$$

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

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

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

$$\mathcal{P}_{RH}(c)=\left\{X\in\mathbb{R}^n \middle| x_n=0,\left|x_i-x_j\right|<1\ \forall\{i,j\}\in c,\left|x_i-x_j\right|>1\ \forall\{i,j\}\in\overline{c}\right\}.$$

Graph Homomorphisms

The method of graph homomorphisms was introduced in [6] for the calculation of the Mayer weight $w_M(b)$ of a 2-connected graph b in the context of hard-core continuum gases in one dimension and was fited in [5] to the context of Ree-Hoover weights. Since $w_M(b)=(-1)^{e(b)}\operatorname{Vol}(\mathcal{P}(b))$, the calculation of $w_M(b)$ is reduced to the calculation of the volume of the polytope $\mathcal{P}(b)$ associated to b. In order to compute this volume, the polytope $\mathcal{P}(b)$ is decomposed into $\nu(b)$ simplices which are all of volume $1/(n-1)!$ and we will have $\operatorname{Vol}(\mathcal{P}(b))=\nu(b)/(n-1)!$. Each simplice is represented by a diagram associated to the integral parts and the relative positions of the fractional parts of the coordinates $x_1,\cdots,x_n$ of points $X\in\mathcal{P}(b)$.

More specifically, to each real number x, they associate his fractional representation, which is a pair (ξ_x,h_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 $h_x=h_y+1$". It mean that 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. Let b a 2-connected graph with vertex set $[n]$, and let $X=(x_1,\cdots,x_n)$ be a point in the polytope $\mathcal{P}(b)$. Let's write (ξ_i,h_i) for the fractional representation of the coordinate x_i of X. For $x_n=0$, it will be convenient to use the special representation $\xi_n=1.0$ and $h_n=-1$. Remarque that the volume of $\mathcal{P}(b)$ is unchanged by removing all hyperplanes $\{x_i-x_j=k\}$, for $k\in\mathbb{Z}$. in consequence, we can assume that all the fractional parts ξ_i are distinct. We get a subpolytope of $\mathcal{P}(b)$ by fixing the "heights" $h_1,h_2,\cdots,h_n$ as well as the relative positions (total order) of the fractional parts $\xi_1, \xi_2, \cdots, \xi_n$. 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 with $\beta(n) = n$. Explicitly, each simplex $\mathcal{P}(h,\beta)$ can be written as

$$\mathcal{P}(h,\beta) = \left\{ (h_1 + \xi_1, \cdots, h_{n-1} + \xi_{n-1}, 0) \middle| 0 < \xi_{\beta^{-1}(1)} < \cdots < \xi_{\beta^{-1}(n-1)} < 1 \right\} \quad (16)$$

and it is shown in [1] that each such simplex is affine-equivalent to the standard simplex

$$\mathcal{P}(0,\mathrm{id}) = \left\{ (\xi_1, \xi_2, \cdots, \xi_{n-1}, 0) \middle| 0 < \xi_1 < \xi_2 < \cdots < \xi_{n-1} < 1 \right\}$$

of volume $1/(n-1)!$.

Note that the simplices (16) are disjoint and each such simplex can be characterized by its centre of gravity

$$X_{h,\beta} = \left(h_1 + \frac{\beta(1)}{n}, h_2 + \frac{\beta(2)}{n}, \cdots, h_{n-1} + \frac{\beta(n-1)}{n}, 0 \right).$$

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 get a configuration in the plane which is an homomorphic image of *b* which represents the subpolytope $\mathcal{P}(h,\beta)$. The above content is summarized in to the form of a proposition:

Proposition 1. ([6]). *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*:

for any edge $\{i,j\}$ of *b*, $\beta(i) < \beta(j)$ implies $h_i = h_j$ or $h_i = h_j + 1$. (17)

Corollary 1. ([6]). *Let b be a* 2*-connected graph and let* $\nu(b)$ *be the number of pairs* (h,β) *such that the condition* (17) *is satisfied. Then the volume of the polytope* $\mathcal{P}(b)$ *is given by*

$$\mathrm{Vol}(\mathcal{P}(b)) = \nu(b)/(n-1)!. \quad (18)$$

Proposition 1 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 2. ([5]). *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*:

for any edge $\{i,j\}$ of b, $\beta(i)<\beta(j)$ implies $h_i=h_j$ or $h_i=h_j+1$. (19)

for any edge $\{i,j\}$ of $\overline{b}$, $\beta(i)<\beta(j)$ implies $h_i\le h_j-1$ or $h_i\ge h_j+2$. (20)

Proposition 3. ([5]). *Let b be a 2-connected graph and let $v_{RH}(b)$ be the number of pairs (h,β) such that conditions* (19) *and* (20) *are satisfied. Then the volume of $\mathcal{P}_{RH}(b)$ is given by*

$$\mathrm{Vol}(\mathcal{P}_{RH}(b))=v_{RH}(b)/(n-1)!. \tag{21}$$

3. Ree-Hoover Weight of New Families of Graphs

In this section, we give other explicit formulas for the Ree-Hoover weight for infinite families of 2-connected graphs. First, we use Ehrhart polynomials to conjectured these formulas from numerical values. We use the techniques of *graph homorphisms* in order to prove these formulas. The weights of 2-connected graphs b are given in absolute value $|w(b)|$, the sign being always equal to $(-1)^{e(b)}$.

Lemma 1. ([5]). *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 $\beta(i)>\beta(j)$.

3.1. The Ree-Hoover Weight of the Graph $K_n\backslash((C_4\cdot\cdot S_2)\cdot S_1)$

Let $(C_4\cdot\cdot S_2)\cdot S_k$ denote the graph obtained by identifying one vertex, with degree three, of the graph $(C_4\cdot\cdot S_2)$ with a center of a k-star. See **Figure 3** for an example.

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

Proposition 4. *For $n\ge 7$, we have*

$$\left|w_{RH}\left(K_n\backslash((C_4\cdot\cdot S_2)\cdot S_1)\right)\right|=\frac{12}{(n-1)(n-2)(n-3)(n-4)(n-5)}. \tag{22}$$

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

According to Lemma 1 there are two possibilities for h:

- $h_1=h_2=h_4=h_5=1$ and $h_n=-1$ and all other $h_i=0$, so that $\beta(5)=1$ and $\beta(3)=2$ and $(\beta(1),\beta(2),\beta(4))$ must be a permutation of $\{3,4,5\}$.
- $h_1=h_2=h_4=h_5=-2$ and all other $h_i=-1$, so that $\beta(5)=n-1$ and $\beta(3)=n-2$ and $(\beta(1),\beta(2),\beta(4))$ must be a permutation of $\{n-3,n-4,n-5\}$.

In each case β can be extended in $(n-6)!$ ways, giving the possible relative positions of the $(n-6)$ x_i (see **Figure 5**). So, there are $2\cdot 3!(n-6)!$ RH-configurations (h,β).

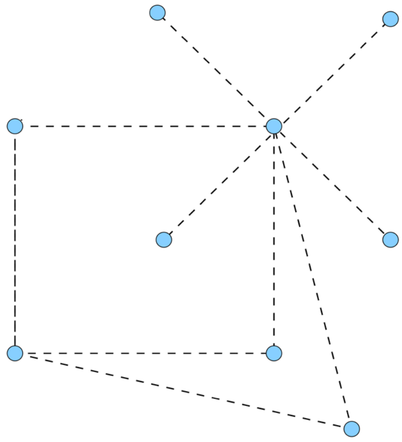

Figure 3. The graph $(C_4 \cdot\cdot S_2) \cdot S_4$.

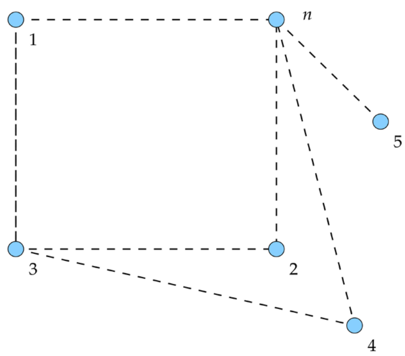

Figure 4. The graph $(C_4 \cdot\cdot S_2) \cdot S_1$.

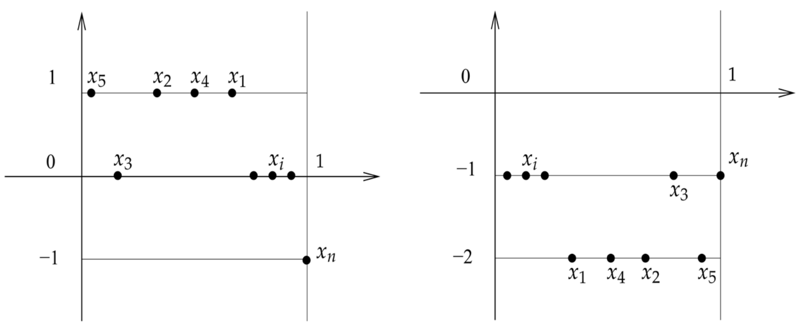

Figure 5. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}\left(K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right) \cdot S_1\right)\right)$.

3.2. The Ree-Hoover Weight of the Graph $K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right) \cdot S_k\right)$

In the general case we have:

Proposition 5. *For* $k \geq 1$, $n \geq k+6$, *we have*

$$\left|w_{RH}\left(K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right) \cdot S_k\right)\right)\right| = \frac{12k!}{(n-1)(n-2)\cdots(n-k-4)}. \tag{23}$$

Proof. We can assume that the missing edges are $\{1,n\}$, $\{2,n\}$, $\{4,n\}$,

$\{3,4\}$, $\{2,3\}$, $\{1,3\}$ and $\{5,n\}$, $\{6,n\}$, $\cdots$, $\{k+4,n\}$ (see **Figure 6**, for the case of $(C_4 \cdot\cdot S_2)\cdot S_2$).

According to Lemma 1 there are two possibilities for h:

- $h_1 = h_2 = h_4 = h_5 = \cdots = h_{k+4} = 1$ and $h_n = -1$ and all other $h_i = 0$, so that $(\beta(5),\beta(6),\beta(7),\cdots,\beta(k+4))$ must be a permutation of $\{1,2,3,\cdots,k\}$ and $\beta(3) = k+1$ and $(\beta(1),\beta(2),\beta(4))$ must be a permutation of $\{k+2,k+3,k+4\}$.
- $h_1 = h_2 = h_4 = h_5 = \cdots = h_{k+4} = -2$ and all other $h_i = -1$, so that $(\beta(5),\beta(6),\beta(7),\cdots,\beta(k+4))$ must be a permutation of $\{n-1,n-2,n-3,\cdots,n-k\}$ and $\beta(3) = n-k-1$ and $(\beta(1),\beta(2),\beta(4))$ must be a permutation of $\{n-k-2,n-k-3,n-k-4\}$.

In each case β can be extended in $(n-k-5)!$ ways, giving the possible relative positions of the $(n-k-5)$ x_i (see **Figure 7**, for the case of $S_2 \cdot C_4 \cdot\cdot S_2$). So, there are $2\cdot 3!k!(n-k-5)!$ RH-configurations (h,β).

We need to use Propositions (6)-(10) to prove Mayer's weight formulas that will be presented in section 4.

Proposition 6. ([5]). For $n \ge 6$, we have

$$\left|w_{RH}\left(K_n \setminus C_4\right)\right| = \frac{8}{(n-1)(n-2)(n-3)}, \tag{24}$$

where C_4 is the unoriented cycle with 4 vertices.

Proposition 7. ([5]). For $k \ge 1$, $n \ge k+3$, we have

$$\left|w_{RH}\left(K_n \setminus S_k\right)\right| = \frac{2k!}{(n-1)(n-2)\cdots(n-k)}, \tag{25}$$

where S_k denote the k-star graph with vertex set $[k+1]$ and edge set $\{\{1,2\},\{1,3\},\cdots,\{1,k+1\}\}$, (see **Figure 8**, for the case of S_3).

Proposition 8. ([5]). For $j \ge k \ge 1$, $n \ge k+j+3$, we have

$$\left|w_{RH}\left(K_n \setminus \left(S_j - S_k\right)\right)\right| = \frac{2k!\,j!}{(n-1)(n-2)\cdots(n-(k+j+1))}, \tag{26}$$

where $S_j - S_k$ denote the graph obtained by joining with a new edge the centers of a j-star and of a k-star. See **Figure 9** for an example.

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

$$\left|w_{RH}\left(K_n \setminus \left(C_4 \cdot S_k\right)\right)\right| = \frac{4k!}{(n-1)(n-2)\cdots(n-(k+3))}, \tag{27}$$

where $C_4 \cdot S_k$ denote the graph obtained by identifying one vertex of the graph C_4 with the center of a k-star. See **Figure 10** for an example.

Proposition 10. ([18]). For $n \ge 7$, we have

$$\left|w_{RH}\left(K_n \setminus \left(C_4 \cdot\cdot S_2\right)\right)\right| = \frac{24}{(n-1)(n-2)(n-3)(n-4)}, \tag{28}$$

where $(C_4 \cdot\cdot S_2)$ denote the graph obtained by identifying two non adjacent vertices of the graph C_4 (the unoriented cycle with 4 vertices) with the extremities of a 2-star (see **Figure 11**).

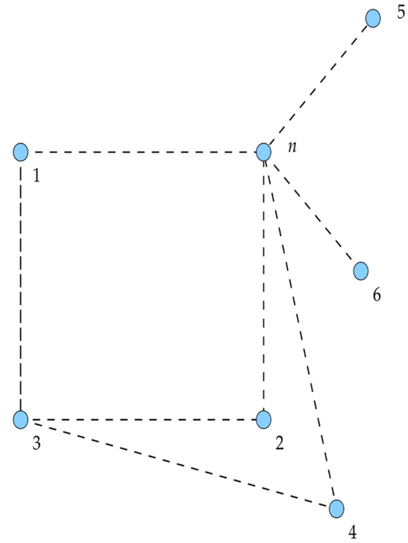

Figure 6. The graph $(C_4 \cdot\cdot S_2)\cdot S_2$.

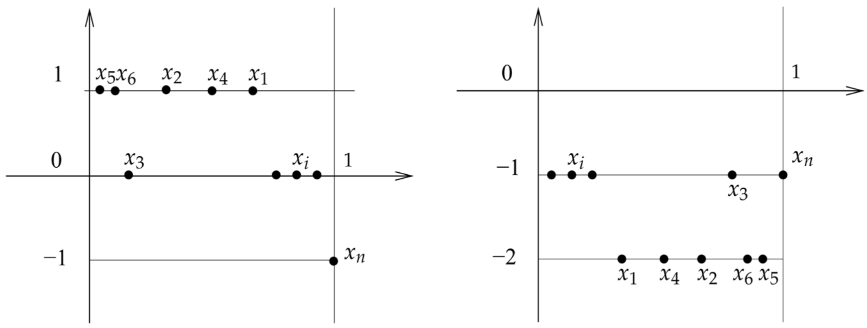

Figure 7. Fractional representation of a simplicial subpolytope of $\mathcal{P}_{RH}\left(K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right)\cdot S_2\right)\right)$.

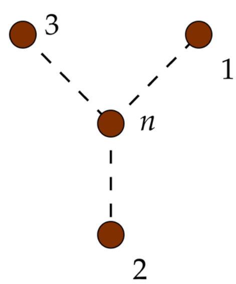

Figure 8. The graph S_3.

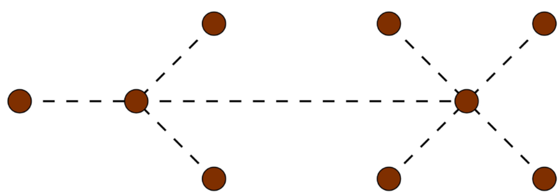

Figure 9. The graph $S_3 - S_4$.

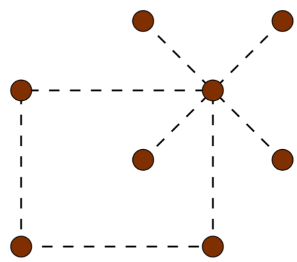

Figure 10. The graph $C_4 \cdot S_4$.

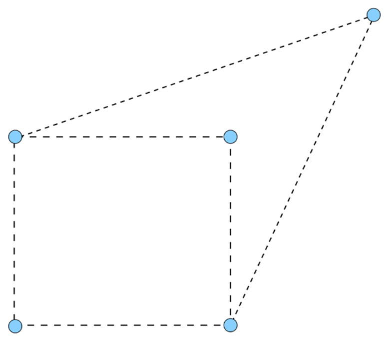

Figure 11. The graph $C_4 \cdot\cdot S_2$.

4. Mayer Weight of New Families of Graphs

Here are some of our results concerning new explicit formulas for the Mayer weight of the previous infinite families of graphs. In this case, the computation of the Mayer weight is more difficult. Instead of using the method of graph homomorphisms, we use the following formula

$$\left|w_M(b)\right| = \sum_{b \subseteq d \subseteq K_n} \left|w_{RH}(d)\right| \tag{29}$$

which is a consequence of (1.11) in the case of hard-core continuum gases in one dimension. Substituting $K_n \setminus g$ and $K_n \setminus k$ for b and d in (29), we have

$$\left|w_M(K_n \setminus g)\right| = \sum_{k \subseteq g} \left|w_{RH}(K_n \setminus k)\right| = \sum_{\tilde{h} \subseteq \tilde{g}} m(\tilde{h}, \tilde{g}) \left|w_{RH}(K_n \setminus h)\right|, \tag{30}$$

where $\tilde{g}$ denotes the unlabelled graph corresponding to g, $\tilde{h}$ runs through the unlabelled subgraphs of $\tilde{g}$ and $m(\tilde{h}, \tilde{g})$ is the number of ways of obtaining $\tilde{h}$ by removing some edges in $\tilde{h}$. We obtain these multiplicities $m(\tilde{h}, \tilde{g})$ by combinatorial arguments.

4.1. The Mayer Weight of the Graph $K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_1)$

Proposition 11. *For* $n \geq 7$, *we have*

$$\begin{aligned} \left|w_M\left(K_n \setminus (C_4 \cdot\cdot S_2) \cdot S_1\right)\right| = n + \frac{14}{n-1} + \frac{48}{(n-1)(n-2)} + \frac{114}{(n-1)\cdots(n-3)} \\ + \frac{156}{(n-1)\cdots(n-4)} + \frac{72}{(n-1)\cdots(n-5)}. \end{aligned} \tag{31}$$

Proof. The over graphs of $K_n \setminus (C_4 \cdot\cdot S_2) \cdot S_1$ whose Ree-Hoover weight is not zero are up to isomorphism of the form: $K_n \setminus C_4$, $K_n \setminus C_4 \cdot S_l$, $1 \le l \le 2$, $K_n \setminus C_4 \cdot\cdot S_2$, $K_n \setminus (C_4 \cdot\cdot S_2) \cdot S_1$, $K_n \setminus S_l$, $1 \le l \le 4$, $K_n \setminus (S_1 - S_l)$, $1 \le l \le 3$, and K_n. Their multiplicities are given by

$$\begin{aligned}
&\left|w_M\left(K_n \setminus (C_4 \cdot\cdot S_2) \cdot S_1\right)\right| \\
&= \left|w_{RH}\left(K_n\right)\right| + 7\left|w_{RH}\left(K_n \setminus S_1\right)\right| + 12\left|w_{RH}\left(K_n \setminus S_2\right)\right| + 5\left|w_{RH}\left(K_n \setminus S_3\right)\right| \\
&\quad + \left|w_{RH}\left(K_n \setminus S_4\right)\right| + 3\left|w_{RH}\left(K_n \setminus C_4\right)\right| + 15\left|w_{RH}\left(K_n \setminus (S_1 - S_1)\right)\right| \\
&\quad + 12\left|w_{RH}\left(K_n \setminus (S_1 - S_2)\right)\right| + 3\left|w_{RH}\left(K_n \setminus (S_1 - S_3)\right)\right| + \left|w_{RH}\left(K_n \setminus (C_4 \cdot\cdot S_2)\right)\right| \\
&\quad + 9\left|w_{RH}\left(K_n \setminus (C_4 \cdot S_1)\right)\right| + 3\left|w_{RH}\left(K_n \setminus (C_4 \cdot S_2)\right)\right| + \left|w_{RH}\left(K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_1)\right)\right|.
\end{aligned}$$

We conclude using Propositions (5) and (6)-(10).

4.2. The Mayer Weight of the Graph $K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_k)$

Proposition 12. *For* $k \ge 1$, $n \ge k+6$, $g_n = K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_k)$, *we have, with the usual convention* $\binom{k+1}{\ell} = 0$ *if* $\ell > k+1$,

$$\begin{aligned}
\left|w_M\left(g_n\right)\right| &= n + \frac{6}{(n-1)} + \frac{60}{(n-1)(n-2)(n-3)(n-4)} \\
&\quad + \frac{24}{(n-1)(n-2)} + \frac{60}{(n-1)(n-2)(n-3)} \\
&\quad + \sum_{l=1}^{k+3}\left[\binom{k+3}{l}\frac{2l!}{(n-1)\cdots(n-l)} + \binom{k+1}{l}\frac{12l!}{(n-1)\cdots(n-l-3)}\right] \\
&\quad + \sum_{l=1}^{k+2}\left[\binom{k}{l-2} + 2\binom{k}{l-1} + \binom{k}{l}\right]\left[\frac{6l!}{(n-1)\cdots(n-l-2)}\right] \\
&\quad + \sum_{l=1}^{k}\binom{k}{l}\left[\frac{12l!}{(n-1)\cdots(n-l-4)}\right].
\end{aligned}$$

Proof. The over graphs of $K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_k)$ whose Ree-Hoover weight is not zero are up to isomorphism of the form: $K_n \setminus S_l$, $1 \le l \le k+3$, $K_n \setminus (C_4 \cdot S_l)$, $1 \le l \le k+1$, $K_n \setminus (S_1 - S_l)$, $1 \le l \le k+2$, $K_n \setminus C_4$, $K_n \setminus (C_4 \cdot\cdot S_2)$, $K_n \setminus ((C_4 \cdot\cdot S_2) \cdot S_l)$, $1 \le l \le k$ and K_n. Their multiplicities are given by

$$\begin{aligned}
\left|w_M\left(g_n\right)\right| &= \left|w_{RH}\left(K_n\right)\right| + 3\left|w_{RH}\left(K_n \setminus S_1\right)\right| + 6\left|w_{RH}\left(K_n \setminus S_2\right)\right| + \left|w_{RH}\left(K_n \setminus S_3\right)\right| \\
&\quad + 3\left|w_{RH}\left(K_n \setminus C_4\right)\right| + 12\left|w_{RH}\left(K_n \setminus S_1 - S_1\right)\right| + 6\left|w_{RH}\left(K_n \setminus S_1 - S_2\right)\right| \\
&\quad + \left|w_{RH}\left(K_n \setminus (C_4 \cdot\cdot S_2)\right)\right| + 3\left|w_M\left(K_n \setminus (C_4 \cdot S_1)\right)\right| \\
&\quad + \sum_{l=1}^{k+1} 3\binom{k+1}{l}\left[\left|w_{RH}\left(K_n \setminus C_4 \cdot S_l\right)\right| + \binom{k}{l}\left|w_{RH}\left(K_n \setminus (C_4 \cdot\cdot S_2) \cdot S_l\right)\right|\right] \\
&\quad + \sum_{l=1}^{k+2} 3\left[\binom{k}{l} + 2\binom{k}{l-1} + \binom{k}{l-2}\right]\left|w_{RH}\left(K_n \setminus S_1 - S_l\right)\right|
\end{aligned}$$

$$+\sum_{l=1}^{k+3}\binom{k+3}{l}\left|w_{RH}\left(K_n \setminus S_l\right)\right|.$$

We conclude using Propositions (5) and (6)-(10).

5. Conclusion

The links between statistical mechanics and combinatorics are more and more numerous as we have seen in this work. In this paper, after recalling the Mayer and Ree-Hoover theory, we presented in Section 2 the method of graph homomorphisms and we have mainly placed ourselves in the context of hard-core continuum gas in one dimension. From various tables that we constructed giving numerical values of Mayer and Ree-Hoover weights of all 2-connected graphs up to size 8, we conjectured explicit formulas for Mayer and Ree-Hoover weights of the family $\left(K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right)\cdot S_1\right)\right)$, $n \geq 7$, and more generally for the family $\left(K_n \setminus \left(\left(C_4 \cdot\cdot S_2\right)\cdot S_k\right)\right)$, $k \geq 1$, $n \geq k+6$. These formulas have been proved in Section 3 by the method of graph homomorphisms for the Ree-Hoover weight and by the linear relations between the two weights for Mayer's weight in Section 4. A similar work was done by the author, see [18], for families of graphs $\left(K_n \setminus \left(C_4 \cdot\cdot S_2\right)\right)$, $n \geq 7$ and $\left(K_n \setminus \left(S_1 \cdot C_4 \cdot\cdot S_2\right)\right)$, $n \geq 7$, and more generally for families $\left(K_n \setminus \left(S_k \cdot C_4 \cdot\cdot S_2\right)\right)$, $k \geq 1$, $n \geq k+6$. These developments pave the way for several future research prospects. For example, the extension of the exact calculation of Mayer's weight and Ree-Hoover's weight for families of graphs $\left(K_n \setminus \left(S_1 \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_1\right)\right)$, $n \geq 8$ and $\left(K_n \setminus \left(S_1 \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_2\right)\right)$, $n \geq 9$ and $\left(K_n \setminus \left(S_2 \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_1\right)\right)$, $n \geq 9$ and more generally for families $\left(K_n \setminus \left(S_1 \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_k\right)\right)$, $k \geq 1$, $n \geq k+6$ and $\left(K_n \setminus \left(S_k \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_1\right)\right)$, $k \geq 1$, $n \geq k+6$, with $\left(S_j \cdot \left(C_4 \cdot\cdot S_2\right)\cdot S_k\right)$ denote the graph obtained by joining with an edge of the graph $C_4 \cdot\cdot S_2$ the centers of a *j*-star and *k*-star.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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