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Mayer and Ree-Hoover weights, graph invariants and bipartite complete graphs

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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. For hard-core continuum gas in one dimension, the explicit computation of these weights for particular graphs is difficult and has been made only for specific families of graphs. We show that the computation of these weights for general graphs cannot be expressed as functions involving only some classical parameters on graphs. Next, we compute the exact Mayer and Ree-Hoover weights of the bipartite complete graphs $K_{m,n}$.

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1 Introduction

The classical formula in statistical mechanics

$$\frac{P}{kT} = \frac{N}{V}, \tag{1}$$

(or $PV = NkT$) for ideal gases has been extended for non ideal gases to an expansion of the form

$$\frac{P}{kT} = \frac{N}{V} + \beta_2\left(\frac{N}{V}\right)^2 + \beta_3\left(\frac{N}{V}\right)^3 + \cdots, \tag{2}$$

called the virial expansion (see [4, 5, 6, 8, 9, 10, 13, 14, 16]), with

$$\beta_n = \frac{1-n}{n!}\sum_{b\in\mathcal{B}[n]} w_M(b), \qquad n \geq 2, \tag{3}$$

where $\mathcal{B}[n]$ is the set of all simple 2-connected graphs (also called blocks) over $[n] = \{1, 2, \ldots, n\}$ and $w_M(b)$ denotes the Mayer weight of the 2-connected graph b. In (1) and (2), P, T, V, N and k respectively denote pressure, temperature, volume, number of particles, and a constant depending on

the gas. In this paper, all graphs are interpreted as sets of edges. Hence, if g is a graph, $\{i,j\} \in g$ means that $\{i,j\}$ is an edge of g.
In the context of hard-core continuum gas in one dimension, the Mayer weight $w_M(g)$ of a connected graph g over $[n]$ is defined by the following multiple integral (see [5, 6, 8]),

$$w_M(g) = (-1)^{e(g)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\}\in g} \chi(|x_i - x_j| < 1) dx_1 \dots dx_{n-1}, \qquad x_n = 0. \tag{4}$$

It is easy to see that

$$w_M(g) = (-1)^{e(g)} \mathrm{vol}(\mathcal{P}(g)), \tag{5}$$

where $e(g)$ denotes the number of edges of g and $\mathrm{vol}(\mathcal{P}(g))$ is the volume of the $(n-1)$-dimensional polytope

$$\mathcal{P}(g) = \{(x_1, \dots, x_n) \in \mathbb{R}^n \mid \forall \{i,j\} \in g, \quad |x_i - x_j| \le 1, \quad x_n = 0\}. \tag{6}$$

An important rewriting of the virial coefficients β_n was performed by Ree and Hoover (see [11, 12]) and later Clisby and McCoy (see [1, 2, 3]) by introducing the Ree-Hoover weight

$$w_{RH}(b) = (-1)^{e(b)} \int_{\mathbb{R}^{n-1}} \prod_{\{i,j\}\in b} \chi(|x_i - x_j| < 1) \prod_{\{i,j\}\in \bar{b}} \chi(|x_i - x_j| > 1) dx_1 \dots dx_{n-1}, \qquad x_n = 0, \tag{7}$$

where $\bar{b} = K_n \backslash b$ is the complementary graph of b. It turns out that (see [6])

$$w_M(b) = \sum_{b \subseteq d \subseteq K_n} (-1)^{e(d)-e(b)} w_{RH}(d), \tag{8}$$

where the sum runs through all graphs d containing b. So that the virial coefficient can be rewritten in the form

$$\beta_n = \frac{1-n}{n!} \sum_{b \in \mathcal{B}[n]} a_n(b) w_{RH}(b), \tag{9}$$

for suitable coefficients $a_n(b)$ called the *star content* of the graph b. The importance of (9) 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 Ehrhart polynomials (see [15]) we have made extensive tables (see [7, 8]) giving the exact values of $w_M(b)$ and $w_{RH}(b)$ for all 2-connected graphs b with at most 8 vertices.
The explicit computation of Mayer or Ree-Hoover weights of particular graphs is very difficult in general and have been made only for certain specific families of graphs (e.g., the complete graphs K_n, the cycle graphs C_n, 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).
In the present paper in the case of hard-core continuum gas in one dimension, we illustrate, in Section 2, the "complexity" of the combinatorial interpretation of $w_M(b)$ and $w_{RH}(b)$ by showing that for a general 2-connected graph b, these weights cannot be expressed as functions involving only certain families of classical graph invariants. In Section 3, we give new explicit formulas for the Mayer and Ree-Hoover weights of the doubly-indexed family $K_{m,n}$ of bipartite complete graphs.

2 Mayer and Ree-Hoover weights versus graph invariants

We illustrate the "complexity" of the combinatorial interpretations of $w_M(b)$ and $w_{RH}(b)$ by showing that for a general 2-connected graph b, these weights cannot be expressed as functions involving only certain subfamilies of the following graph invariants:
Sequence of degrees, $\delta(b)$; number of edges, $e(b)$; number of vertices, $n(b)$; star content, $a_n(b)$; number of covering trees, $\gamma(b)$; order of the automorphism group, $\mathrm{aut}(b)$; Mayer polytope volume, $\mathrm{vol}_M(b)$; Ree-Hoover polytope volume, $\mathrm{vol}_{RH}(b)$; $w_M(b)$ (in the case of $w_{RH}(b)$); $w_{RH}(b)$ (in the case of $w_M(b)$).
More precisely, using the GraphTheory Maple Package and the above mentioned tables [7] for 2-connected graphs having up to 8 vertices we give explicit examples of 2-connected graphs g_1, g_2 for which $w_M(g_1) \neq w_M(g_2)$ or $(w_{RH}(g_1) \neq w_{RH}(g_2))$ having the same set of invariants taken from the above list. In the computer search, involving 7662 graphs, all sublists of invariants have been tested and we kept only the maximal ones.

2.1 The Mayer case

THEOREM 2.1 *There is no function $f_1(x_1, x_2, \cdots, x_6)$ such that*

$$w_M(b) = f_1\left(n(b), \delta(b), \gamma(b), e(b), w_{RH}(b), \mathrm{aut}(b)\right)$$

and no function $f_2(x_1, x_2, \cdots, x_6)$ such that

$$w_M(b) = f_2(n(b), \mathrm{vol}_{RH}(b), \mathrm{aut}(b), \mathrm{vol}_M(b), w_{RH}(b), a_n(b))$$

for every 2-connected graph b.

Proof.
a) The two graphs b_1 and b_2 of Figure 1 have distinct Mayer weights

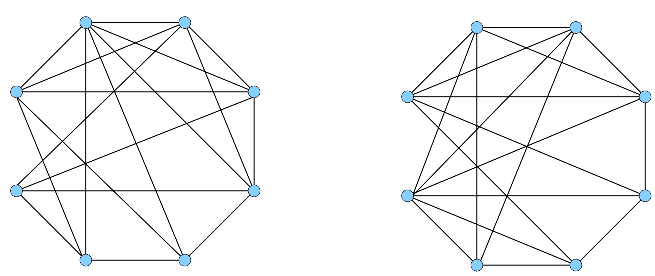

Figure 1: $w_M(b_1) = -\frac{3856}{315} \neq w_M(b_2) = -\frac{1103}{90}$

but both have the same:

- Number of vertices: 8,
- Sequence of degrees: $[6, 5^4, 4^3]$,
- Number of covering trees: 12852,
- Number of edges: 19,
- Ree-Hoover weight: 0,
- Order of the automorphism group: 2.

b) The two graphs b_1 and b_2 of Figure 2 have distinct Mayer weights

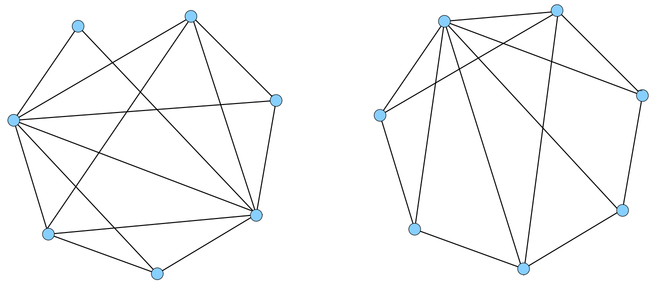

Figure 2: $w_M(b_1) = \frac{2251}{180} \neq w_M(b_2) = -\frac{2251}{180}$

but both have the same:

- Number of vertices: 7,
- Ree-Hoover polytope volume: 0,
- Order of the automorphism group: 4,
- Mayer polytope volume: $\frac{2251}{180}$,
- Ree-Hoover weight: 0,
- Star content: 0.

□

2.2 The Ree-Hoover case

THEOREM 2.2 *There is no function* $h_1(x_1, x_2, \cdots, x_6)$ *such that*

$$w_{RH}(b) = h_1(n(b), w_M(b), \mathrm{aut}(b), e(b), \gamma(b), a_n(b)),$$

no function $h_2(x_1, x_2, \cdots, x_5)$ *such that*

$$w_{RH}(b) = h_2(n(b), \delta(b), a_n(b), e(b), \mathrm{aut}(b))$$

and no function $h_3(x_1, x_2, \cdots, x_4)$ *such that*

$$w_{RH}(b) = h_3(n(b), \mathrm{aut}(b), \mathrm{vol}_{RH}(b), a_n(b))$$

for every 2-connected graph b.

Proof.

a) The two graphs b_1 and b_2 of Figure 3 have distinct Ree-Hoover weights

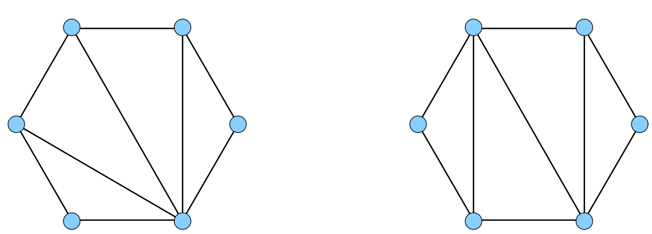

Figure 3: $w_{RH}(b_1) = 0 \neq w_{RH}(b_2) = -\frac{1}{30}$

but both have the same:

- Number of vertices: 6,
- Mayer weight: $-\frac{169}{15}$,
- Order of the automorphism group: 2,
- Number of edges: 9,
- Number of covering trees: 55,
- Star content: 0.

b) The two graphs b_1 and b_2 of Figure 4 have distinct Ree-Hoover weights

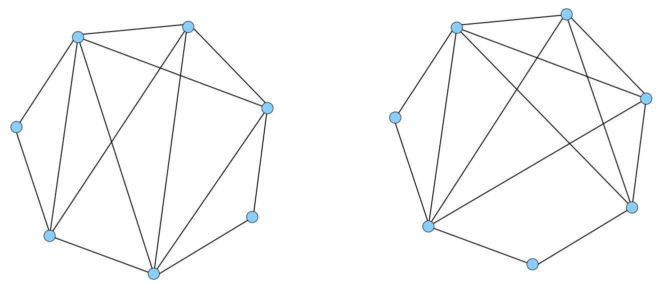

Figure 4: $w_{RH}(b_1) = -\frac{1}{360} \neq w_{RH}(b_2) = 0$

but both have the same:

- Number of vertices: 7,
- Sequence of degrees: $[5^2, 4^3, 2^2]$,
- Star content: 0.
- Number of edges: 13,
- Order of the automorphism group: 2,

c) The two graphs b_1 and b_2 of Figure 5 have distinct Ree-Hoover weights

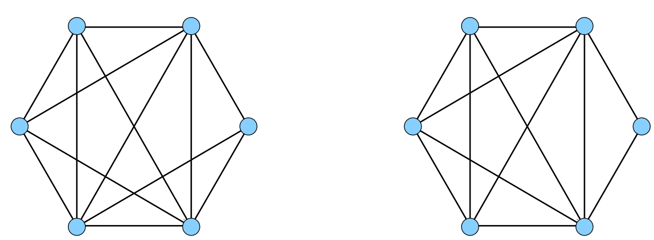

Figure 5: $w_{RH}(b_1) = -\frac{1}{5} \neq w_{RH}(b_2) = \frac{1}{5}$

but both have the same:

- Number of vertices: 6,
- Order of the automorphism group: 12,
- Ree-Hoover polytope volume: $\frac{1}{5}$,
- Star content: 0.

□

3 Complete bipartite graphs $K_{m,n}$ and Beta functions

We now compute the Mayer and Ree-Hoover weights of the 2−parameter family $K_{m,n}$ of bipartite graphs (see Figure 6).
Using Maple and Ehrhart polynomials we made tables (see [7]) from which the following result was first conjectured.

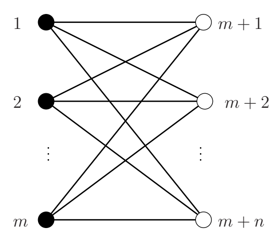

Figure 6: The graph $K_{m,n}$

THEOREM 3.1 *In the context of hard-core continuum gas in one dimension, the Mayer and Ree-Hoover weights of the bipartite graph $K_{m,n}$ are given by*

$$w_M(K_{m,n}) = (-1)^{mn} \cdot \frac{2^{m+n-1} m! n!}{(m+n-1)!}, \quad m,n \geq 1, \tag{10}$$

$$w_{RH}(K_{m,n}) = \begin{cases} 2, & \text{if} \quad m=n=1, \\ 1, & \text{if} \quad \{m,n\}=\{1,2\}, \\ 0, & \text{if} \quad m=1, n \geq 3 \ \text{ or } \ m,n>1. \end{cases} \tag{11}$$

Proof. Consider a complete bipartite graph $K_{m,n}$ built on $[m]$, $[n]$ and introduce variables x_i for $i \in [m]$ and y_j for $j \in [n]$. Formula (4) defining the Mayer weight takes the form

$$w_M(K_{m,n}) = (-1)^{mn} \int_{\mathbb{R}^{m+n-1}} \prod_{\substack{i \in [m] \\ j \in [n]}} \chi(|x_i - y_j| < 1) dx_1 \ldots dx_m dy_1 \ldots dy_{n-1}, \quad y_n = 0. \tag{12}$$

This integral is evaluated in several steps in the following way:

$$\begin{aligned}
w_M(K_{m,n}) &= (-1)^{mn}\int_{\mathbb{R}^{m+n-1}} \prod_{i\in[m]} \chi(|x_i|<1) \prod_{\substack{i\in[m]\\ j\in[n-1]}} \chi(|x_i-y_j|<1)dx_1\dots dx_m dy_1\dots dy_{n-1} \\
&= (-1)^{mn}\underbrace{\int_{-1}^{1}\cdots\int_{-1}^{1}}_{m} \left(\int_{\mathbb{R}^{n-1}} \prod_{\substack{i\in[m]\\ j\in[n-1]}} \chi(|x_i-y_j|<1)dy_1\dots dy_{n-1}\right) dx_1\dots dx_m \\
&= (-1)^{mn}\underbrace{\int_{-1}^{1}\cdots\int_{-1}^{1}}_{m} ((\min x_i+1)-(\max x_i-1))^{n-1}\, dx_1\dots dx_m \\
&= (-1)^{mn}\underbrace{\int_{-1}^{1}\cdots\int_{-1}^{1}}_{m} (2-(\max x_i-\min x_i))^{n-1}\, dx_1\dots dx_m.
\end{aligned}$$

Since,

$$\begin{aligned}
\prod_{\substack{i\in[m]\\ j\in[n-1]}} \chi(|x_i-y_j|<1)=1 \quad &\Leftrightarrow \quad \forall i\in[m], \forall j\in[n-1] : -1<y_j-x_i<1 \\
&\Leftrightarrow \quad (y_1,y_2,\dots,y_{n-1})\in[\max x_i-1, \min x_i+1]^{n-1}.
\end{aligned}$$

Making the change of variables $x_i = z_i - 1$, then $\max x_i - \min x_i = \max z_i - \min z_i$ and

$$w_M(K_{m,n}) = (-1)^{mn}\underbrace{\int_{0}^{2}\cdots\int_{0}^{2}}_{m} (2-(\max z_i-\min z_i))^{n-1}\, dz_1\dots dz_m.$$

We can assume that the variables z_i are distinct (since the set where there is equality has measure zero). We have m choices for $\max z_i$ and $m-1$ choices for $\min z_i$. By symmetry, we can assume that

$$\min z_i = z_1 \quad \text{and} \quad \max z_i = z_2.$$

We then have,

$$z_1 < z_k < z_2, \quad \text{for} \quad k=3,4,\dots,m.$$

Hence,

$$\begin{aligned} w_M(K_{m,n}) &= (-1)^{mn} m(m-1) \underbrace{\int_0^2 \cdots \int_0^2}_{m} (2-(z_2-z_1))^{n-1} \chi(z_1<z_2) \\ &\qquad \cdot \prod_{\nu=3}^{m} \chi(z_1<z_\nu<z_2) dz_1 \ldots dz_m \\ &= (-1)^{mn} m(m-1) \int_0^2 \int_0^2 (2-(z_2-z_1))^{n-1} \chi(z_1<z_2)(z_2-z_1)^{m-2} dz_1 dz_2 \\ &= (-1)^{mn} m(m-1) \int_0^2 \int_{z_1}^2 (2-(z_2-z_1))^{n-1} (z_2-z_1)^{m-2} dz_2 dz_1. \end{aligned}$$

Now let $z_2 = x + z_1$, then

$$\begin{aligned} w_M(K_{m,n}) &= (-1)^{mn} m(m-1) \int_0^2 \left(\int_0^{2-z_1} (2-x)^{n-1} x^{m-2} dx \right) dz_1 \\ &= (-1)^{mn} m(m-1) \int_0^2 \left(\int_0^{2-x} (2-x)^{n-1} x^{m-2} dz_1 \right) dx \\ &= (-1)^{mn} m(m-1) \int_0^2 (2-x)^{n} x^{m-2} dx. \end{aligned}$$

Writing $x = 2t$, gives

$$\begin{aligned} w_M(K_{m,n}) &= (-1)^{mn} m(m-1) \cdot 2^{m+n-1} \int_0^1 t^{m-2} (1-t)^n \, dt \\ &= (-1)^{mn} m(m-1) \cdot 2^{m+n-1} \cdot B(m-1, n+1) \\ &= (-1)^{mn} \cdot \frac{2^{m+n-1} m! n!}{(m+n-1)!}, \end{aligned}$$

where $B(\alpha,\beta) = \int_0^1 t^{\alpha-1} (1-t)^{\beta-1} \, dt$ denotes the classical Beta function.
The first two cases of (11) follow directly from the definition (7) of the Ree-Hoover weight. For the remaining cases we need the following definition and Theorem 3.3 below taken from [6].

Definition 3.2 [6] 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

$$g' = g \cap K_{U'}, \tag{13}$$

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

Theorem 3.3 [6] *The Ree-Hoover weight of a 2-connected graph g of size n is zero if g satisfies one of the following conditions,*

$$g \text{ is chordal } : \ C_k \,\overline{\subseteq}\, g, \quad k \geq 4, \tag{14}$$

$$\text{or } g \text{ is claw-free } : \ S_3 \,\overline{\subseteq}\, g, \tag{15}$$

where S_3 is the 3-star graph (see Figure 7) and C_k is the cycle on k elements.

Proof. See [6]. □

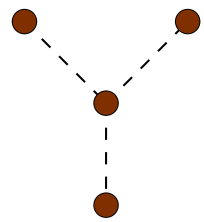

Figure 7: The graph S_3

To continue the proof of Theorem 3.1 let now $m = 1$ and $n \geq 3$. Then $K_{m,n}$ contains S_3 as an induced subgraph (see Figure 8) so that $w_{RH}(K_{m,n}) = 0$ by Theorem 3.3.

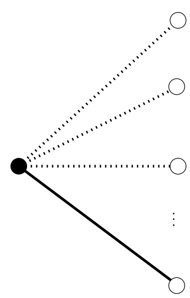

Figure 8: The graph $K_{1,n}$, $n \geq 3$

Finally, let $m, n > 1$. Then $K_{m,n}$ contains C_4 as an induced subgraph (see Figure 9) so that $w_{RH}(K_{m,n}) = 0$ by Theorem 3.3.

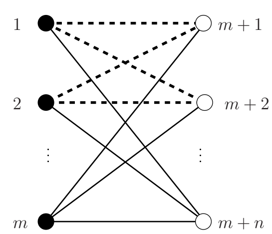

Figure 9: The graph $K_{m,n}$, $m, n > 1$

□

Remark 3.4 From Formula (10), we obtain the recurrences

$$w_M(K_{n,n-1}) = (-1)^n w_M(K_{n,n-2}), \quad n \geq 4, \tag{16}$$

and

$$w_M(K_{m,n+1}) = (-1)^m \frac{2(n+1)}{n+m} w_M(K_{m,n}). \tag{17}$$

PROPOSITION 3.5 *In the more general case of the complete multipartite graph, $K_{n_1,n_2,\cdots,n_k}$, we have*

$$w_{RH}(K_{n_1,n_2,\cdots,n_k}) = \begin{cases} k, & \text{if} \quad \forall i, \quad n_i = 1, \\ \frac{2}{k}, & \text{if} \quad \exists i, \quad n_i = 2, \quad \forall j \neq i, \quad n_j = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{18}$$

Proof. The first case of (18) follows from the known fact (see [6] and [8]) that $w_{RH}(K_k) = w_M(K_k) = k$ since $K_{1,1,\cdots,1} = K_k$.
The second case of (18) follows from the known fact (see [6]) that $w_{RH}(K_{k+1}\backslash e) = \frac{2}{k}$ since $K_{2,1,\cdots,1} = K_{k+1}\backslash e$, where $K_{k+1}\backslash e$ is the complete graph on $k+1$ vertices in which one edge is removed.
The proof of the last case of (18) is similar to the corresponding case in the proof of Theorem 3.1. □

The Mayer weight of complete multipartite graphs is much more complicated. The natural extension

$$2^{n_1+n_2+\cdots+n_k-1} n_1! n_2! \cdots n_k! / (n_1+n_2+\cdots+n_k-1)! \tag{19}$$

of Formula (10) does not give the Mayer weight $w_M(K_{n_1,n_2,\cdots,n_k})$. For example, $w_M(K_{1,1,1}) = w_M(K_3) = 3$, while formula (19) gives the value 2.
For $k \geq 3$, the computation of $w_M(K_{n_1,n_2,\cdots,n_k})$ is left open.

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