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LETTER TO THE EDITOR

The Gaussian model for fluids and covering a graph by spanning trees

Ron M Adin†‡

Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

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Abstract. A certain power series, arising in the Gaussian model for fluids, has been conjectured to reduce to a polynomial when the dimension parameter is a negative even integer. This conjecture is confirmed here, using a graph-theoretical interpretation of the coefficients.

The Mayer cluster series for an imperfect fluid,

$$f_d(z)=\sum_{n=1}^{\infty} b_n(d)z^n \tag{1}$$

expresses thermodynamic quantities (for example, pressure) in terms of the activity z of the d-dimensional fluid. Under the continuum Gaussian model for purely repulsive interactions, the coefficients $b_n(z)$ (the Mayer cluster integrals) may be explicitly represented as

$$b_n(d)=\frac{2^{n-1}}{n!}\sum_k(-1)^k\sum_{c\geqslant 1} c^{-d/2}g(n,k,c). \tag{2}$$

Here $g(n,k,c)$ is the number of graphs with k edges on n labelled vertices that have complexity c. Recall that the complexity of a graph is the number of spanning trees it has, and is therefore positive if and only if the graph is connected.

It has recently been noted that consideration of this model for unconventional values of the parameters may add to the understanding of its properties. In particular, numerical evidence has led Baram and Luban [1] to conjecture that if d is a negative even integer then $b_n(d)=0$ for all $n>|d|$, so that the Mayer series reduces to a polynomial. This conjecture will be proved here, together with some additional properties of the numbers $b_n(d)$ for negative even values of d. In particular, these numbers are found to have a sign-pattern of period 4 (as opposed to period 2 for positive values of d), and they are also always integers (even after the division by $n!$). The main results are summarized in

Theorem 1. Let d be a negative even integer. Then

(i) $b_n(d)\neq 0$ exactly for $1\leqslant n\leqslant |d|$.
(ii) For $1\leqslant n\leqslant |d|$, $b_n(d)>0$ iff n is congruent to 0 or 1 modulo 4.
(iii) $b_1(d),\ldots,b_{|d|}(d)$ are integers.

† Research carried out during a visit to the Institute of Mathematics and Computer Science, Hebrew University, Jerusalem, Israel.
‡ e-mail: radin@math.mit.edu

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(iv) The first four coefficients are

$$b_1(d)=1 \tag{3}$$

$$b_2(d)=-1 \tag{4}$$

$$b_3(d)=-2(3^{m-1}-1) \tag{5}$$

$$b_4(d)=\tfrac{1}{3}(16^m-6\times 8^m+3\times 4^m+12\times 3^m-16) \tag{6}$$

where $m=-d/2$.

Most of these results are consequences of the following observation.

Lemma 2. If m is a positive integer then

$$b_n(-2m)=(-1)^{\binom{n}{2}}2^{n-1}\frac{t_m(n)}{n!} \tag{7}$$

where $t_m(n)$ is the number of m-tuples $(T_1,\ldots,T_m)$ of spanning trees of the complete graph on n vertices, which cover together all the edges of the complete graph. (The T_i need not be distinct.)

Denote by $\mathcal{T}_m(n)$ the set of m-tuples mentioned in lemma 2 (so that $\mathcal{T}_m(n)$ has $t_m(n)$ elements). Another useful result is

Lemma 3. A permutation π of the vertices of K_n that preserves an m-tuple in $\mathcal{T}_m(n)$ is necessarily an involution, i.e. π^2 is the identity permutation.

Proof of lemma 2. Denote by $\mathcal{T}(G)$ the set of all spanning trees of a graph G, and let $\mathcal{T}(n)=\mathcal{T}(K_n)$, where K_n is the complete graph on n vertices. Let $\#S$ denote the number of elements of a finite set S. Then

$$\frac{n!}{2^{n-1}}b_n(-2m)=\sum_k(-1)^k\sum_{c\geq 1}c^m g(n,k,c)$$

$$=\sum_k(-1)^k\#\{(G,T_1,\ldots,T_m)|G \text{ is a subgraph of } K_n \tag{8}$$

$$\text{with } k \text{ edges, and } T_1,\ldots,T_m\in\mathcal{T}(G)\} \tag{9}$$

$$=\sum_{T_1,\ldots,T_m\in\mathcal{T}(n)}\sum_k(-1)^k\#\{G|G \text{ is a subgraph of } K_n$$

$$\text{that contains } T_1,\ldots,T_m \text{ and has } k \text{ edges}\}. \tag{10}$$

The latter equality is obtained by changing the order of summation.

Let $E(G)$ denote the set of edges of a graph G. Given spanning trees $T_1,\ldots,T_m\in\mathcal{T}(n)$, let

$$U=\bigcup_{i=1}^m E(T_i). \tag{11}$$

Then

$$\sum_k(-1)^k\#\{G|G \text{ is a subgraph of } K_n \text{ that contains } T_1,\ldots,T_m \text{ and has } k \text{ edges}\}$$

$$=\sum_k(-1)^k\#\{E\,|\,U\subseteq E\subseteq E(K_n), \#E=k\} \tag{12}$$

$$=(-1)^{\#U}(1-1)^{\#E(K_n)-\#U} \tag{13}$$

$$=\begin{cases}(-1)^{\#E(K_n)} & \text{if } U=E(K_n)\\ 0, & \text{otherwise.}\end{cases} \tag{14}$$

It follows that the non-zero summands in expression (10) above correspond to instances of $U = E(K_n)$, i.e., to m-tuples of trees $(T_1, .., T_m)$ that cover together all the edges of K_n. The number of such m-tuples is precisely $t_m(n)$, as defined above, and each of them contributes $(-1)^{\# E(K_n)} = (-1)^{\binom{n}{2}}$ to the sum. □

Proof of theorem 1. Assume throughout that $d = -2m$ for a positive integer m.

(i) By lemma 2, $b_n(d) = 0$ unless it is possible to cover the complete graph on n vertices by m of its spanning trees, allowing repetitions. Since there are $\binom{n}{2}$ edges in the complete graph and $n-1$ edges in each tree, it is necessary for $b_n(d) \neq 0$ to have

$$m \geqslant \frac{1}{n-1}\binom{n}{2} = \frac{n}{2} \tag{15}$$

that is

$$n \leqslant 2m = |d|. \tag{16}$$

To show that this condition is also sufficient, one must show that K_n may be covered by m spanning trees for any $1 \leqslant n \leqslant 2m$. It is enough to show this for $n = 2m$, since a covering of K_n for smaller n may be obtained from a covering of K_{2m} by deleting $2m - n$ vertices and completing the 'remains' of each spanning tree of K_{2m}, in an arbitrary fashion, to a spanning tree of K_n. Finally, to exhibit an explicit covering of K_{2m} by m spanning trees (actually, by m edge-disjoint Hamiltonian paths), label the vertices by the numbers $0, \ldots, 2m-1$. Let T_1 (see figure 1) be the path consisting of the $2m-1$ edges

$$\begin{aligned}&\{0, m\}\\ &\{m, 1\}, \{1, m-1\}, \{m-1, 2\}, \{2, m-2\}, \ldots\\ &\{0, m+1\}, \{m+1, 2m-1\}, \{2m-1, m+2\}, \{m+2, 2m-2\}, \ldots.\end{aligned} \tag{17}$$

The other paths $T_2, \ldots, T_m$ are obtained from T_1 by cyclic rotations: To get T_i, add $i-1$ to the label of each vertex in the description of T_1, computing modulo $2m$. It is easy to see that each edge of K_{2m} is covered by exactly one of the trees $T_1, \ldots, T_m$.

(ii) The binomial coefficient $\binom{n}{2}$ is even iff n is congruent to 0 or 1 modulo 4.

(iii) Consider again the set $\mathcal{T}(n)$ of all spanning trees of K_n, together with the set of m-tuples

$$\mathcal{T}_m(n) = \{(T_1, \ldots, T_m) | T_1, \ldots, T_m \in \mathcal{T}(n)\}. \tag{18}$$

The symmetric group S_n, consisting of all permutations of n elements, acts naturally on the vertices of K_n, and therefore also on $\mathcal{T}(n)$ and $\mathcal{T}_m(n)$. This action separates

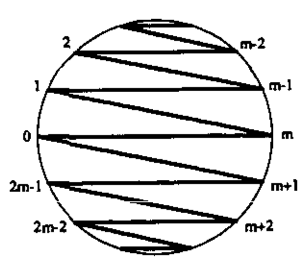

Figure 1. T_1, a spanning tree of K_{2m}.

$\mathscr{T}_m(n)$ into equivalence classes, or orbits. If this action were fixed-point free, each orbit would contain exactly $n!$ elements, and therefore $t_m(n) = \#\mathscr{T}_m(n)$ would be divisible by $n!$. This is not always the case, as the following example shows.

Example. Take $n = 4$, and label the vertices of K_4 by 1 through 4. Let $m = 2$, and consider the spanning trees

$$T_1 = \{12, 23, 14\} \tag{19}$$

$$T_2 = \{13, 34, 24\}. \tag{20}$$

Then T_1 and T_2 cover all the edges of K_4 (see figure 2), and are both invariant under the permutation $(12)(34) \in S_4$. The orbit of (T_1, T_2) in $\mathscr{T}_2(4)$ contains only 12 elements. (Note that we consider *ordered* m-tuples of trees.)

Nevertheless, we claim that the symmetry group of each m-tuple in $\mathscr{T}_m(n)$ cannot be too large. This is essentially the content of lemma 3, which was stated above and is restated here with a proof.

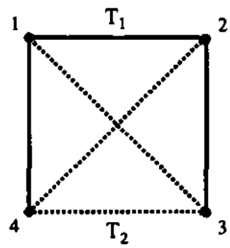

Figure 2. An invariant covering of K_4.

Lemma 3. A permutation π of the vertices of K_n that preserves an m-tuple in $\mathscr{T}_m(n)$ is necessarily an involution, i.e. π^2 is the identity permutation.

Proof. Let $\pi \in S_n$ preserve an m-tuple $(T_1, \ldots, T_m) \in \mathscr{T}_m(n)$, and express π as a product of disjoint cycles. Assuming that π is not an involution, one of its cycles—say $(v_1, \ldots, v_p)$—has length $p \geqslant 3$. Since the trees $T_1, \ldots, T_m$ cover all the edges of the complete graph, at least one of them—say T_i—contains the edge $\{v_1, v_2\}$. Since T_i is π-invariant, it must also contain the edges $\{v_2, v_3\}, \{v_3, v_4\}, \ldots, \{v_p, v_1\}$. This is clearly impossible, since a tree cannot contain any cycle. □

Returning now to the proof of theorem 1, we see that the stabilizer of any m-tuple in $\mathscr{T}_m(n)$ is a subgroup G of S_n that contains involutions only. By the well-known theorems of Lagrange and Cauchy [4, pp 35, 74], the size of G must be a power of 2 that divides $n!$. Let $2^{q_2(n)}$ be the largest power of 2 that divides $n!$. Then

$$q_2(n) = \sum_{i=1}^{\infty} \lfloor n/2^i \rfloor < \sum_{i=1}^{\infty} n/2^i = n \tag{21}$$

and since $q_2(n)$ is an integer, it does not exceed $n-1$. The size of the stabilizer G therefore divides 2^{n-1}, and the corresponding orbit size is an integral multiple of $n!/2^{n-1}$. The sum of all orbit sizes is $t_m(n)$, and therefore the number

$$b_n(-2m) = \pm\frac{2^{n-1}}{n!}\,t_m(n) \tag{22}$$

is an integer.

(iv) Direct computation, using the original definition of the coefficients $b_n(d)$ in equation (2) above. □

Remarks

1. The fact that $t_m(n)/n!$ (without multiplying by an appropriate power of 2) is not always an integer is evident from the numerical values computed in [1], e.g.

$$b_4(-4)=4 \qquad (\text{so } t_2(4)/4! = 1/2) \tag{23}$$

or

$$b_6(-6)=-2944 \qquad (\text{so } t_3(6)/6! = -1977/16). \tag{24}$$

In fact, the formula for $b_4(-2m)$ in theorem 1 shows that $t_m(4)/4!$ is a non-integer whenever it is non-zero (i.e. for $m \geqslant 2$).

2. The actual power of 2 needed to turn $t_m(n)/n!$ into an integer is, in fact, much smaller than the crude estimate $n-1$. For one thing, the function $q_2(n)$ used in the above proof attains its upper bound of $n-1$ if and only if n is a power of 2, since, for $2^k < n < 2^{k+1}$,

$$q_2(n) = \sum_{i=1}^{k} \lfloor n/2^i \rfloor \leqslant \sum_{i=1}^{k} n/2^i = n - n/2^k < n-1 \tag{25}$$

whereas

$$q_2(2^k) = 2^{k-1} + 2^{k-2} + \ldots + 1 = 2^k - 1. \tag{26}$$

Moreover, let $2^{p_2(n)}$ denote the size of the largest subgroup of S_n that contains involutions only. (Note that such a group must be commutative.) Then one has, in fact,

$$p_2(n) = \lfloor n/2 \rfloor \leqslant q_2(n) \leqslant n-1. \tag{27}$$

The inequality $p_2(n) \geqslant \lfloor n/2 \rfloor$ follows from an explicit construction: partition the n vertices into $\lfloor n/2 \rfloor$ pairs (plus a singleton, if n is odd), and consider the group of all the permutations (necessarily involutions) that map each vertex to itself or to its mate in the pairing. The reverse inequality $p_2(n) \leqslant \lfloor n/2 \rfloor$ follows from the following argument (due to R Stanley): it is easy to see if a commutative group acts on a set of size k as a *transitive* permutation group (assuming the action is faithful), then this group has exactly k elements. Therefore, if G is a subgroup of S_n consisting of involutions only, we may consider the various G-orbits (whose sizes add up to n) and conclude that the size of G does not exceed the product of the orbit-sizes. The product of integers with a given sum is maximized if almost all of them are equal to 3, but since the sizes in our case are all powers of 2 it follows that the maximal product is obtained when there are orbits of size 2 (or 4), plus one orbit of size 1 if n is odd. This maximal product is $2^{\lfloor n/2 \rfloor}$.

3. The results of this letter hold in a more general context: if one defines $g(G, k, c)$ to be the number of subgraphs of a given graph G which have k edges and complexity c, and defines $b_G(d)$ by the obvious analogue of formula (2) above (which is the special case $G = K_n$), then the appropriate analogue of lemma 2 will still hold. In particular, $b_G(-2m) = 0$ (for a positive integer m) if and only if m is less than $m(G)$, the minimal number of spanning trees needed to cover all the edges of G. For example, the two-component system discussed in [2] corresponds to the complete bipartite graph K_{n_1,n_2}, with n_1 vertices of one colour, n_2 vertices of another colour, and edges connecting any two vertices of distinct colours. The conjecture of [2], concerning the vanishing cluster integrals in this case, amounts to the claim that

$$m(K_{n_1,n_2}) > \tfrac{1}{2}\min(n_1, n_2). \tag{28}$$

The verification of this conjecture is now straightforward, using the same edge-counting argument as in the proof of theorem 1(i): m spanning trees cover at most $m(n_1 + n_2 - 1)$ edges, whereas the graph K_{n_1,n_2} has $n_1 n_2$ edges. Assuming that $n_1 \leqslant n_2$, it follows that

$$m(K_{n_1,n_2}) \geqslant \frac{n_1 n_2}{n_1 + n_2 - 1} > \frac{n_1 n_2}{2n_2} = \frac{n_1}{2} \tag{29}$$

as claimed.

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