Dimer entropy of a graph and a positivity property, preliminary version

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Abstract

The entropy of a monomer-dimer system on an infinite bipartite lattice can be written as a mean-field part plus a series expansion in the dimer density. In a previous paper it has been conjectured that all coefficients of this series are positive. Analogously on a connected regular graph with v vertices, the “entropy” of the graph $\ln N(i)/v$, where $N(i)$ is the number of ways of setting down i dimers on the graph, can be written as a part depending only on the count of the dimer configuration over the completed graph plus a Newton series in the dimer density on the graph. In this paper, we investigate for which connected regular graphs all the coefficients of the Newton series are positive (for short, these graphs will be called positive). In the class of connected regular bipartite graphs, up to $v = 20$, all the non positive graphs have vertices of degree 3. From $v = 14$ to $v = 28$, and degree 3, a few violations of the positivity occur, but their frequency decreases with increasing v. We conjecture that for each degree r the frequency of violations, in the class of the $r-$regular bipartite graphs, goes to zero as v tends to infinity.

This graph-positivity property can be extended to non-regular or non-bipartite graphs.

We have examined a large number of rectangular grids of size $N_x \times N_y$ both with open and periodic boundary conditions. We have observed positivity violations only for $min(N_x, N_y) = 3$ or 4.

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I. INTRODUCTION

For periodic cubical d-dimensional lattices with even length sides, the number of dimer configurations covering a fraction p of the vertices (called "matchings" of the lattice graph in the language of graph theory) has long been studied. As the number of vertices v tends to infinity, the number of distinct dimer configurations grows[1] as $\exp(v\lambda_d(p))$, where $\lambda_d(p)$ is called the dimer entropy and p is the dimer density. In Ref.[2], the entropy has been written as the sum of a mean field term and of a series expansion in the dimer density, computed through order 6; in Refs.[3,4] this series has been extended at least through the order 20. More precisely, for lattices of dimension $2 \leq d \leq 4$ the first 24 coefficients were derived[3,4], while 20 coefficients have been obtained for all $d > 4$ (in $d = 5, 6$ respectively $22, 21$ coefficients have been computed). In the case of $d = 1$, all coefficients are positive and have long been known. It is striking that, for any integer d, all the series coefficients that we could compute, are positive. This led us to conjecture[4] that: *for all (hyper)-cubical lattices the series coefficients are all positive.* Moreover, after examining the series coefficients for various non-square bipartite lattices, we were led to extend the conjecture to all bipartite lattices (i.e. to the lattices in which the sites can be divided into even and odd, such that no edge connects two vertices with the same parity).

We observe that, in analogy with the case of infinite bipartite lattices, on a connected simple undirected regular bipartite graph G with set of vertices V and set of edges E, the "graph dimer entropy" $\ln N(i)/v$ - where $N(i)$ is the number of ways of setting down i dimers on the graph and $v = |V|$ is the number of vertices of the graph - can be written as a part depending on the dimer configurations counting over the completion of the graph and a Newton expansion in the dimer density on the graph. If all the coefficients of the Newton series are positive, we shall say that the graph satisfies the *graph-positivity* property. For not too large number of vertices v, we have generated *all* regular (bi)connected bipartite graphs (RBB graphs from now on) using the *Nauty* program[5] via the *Sage* interface[6]. In examining all RBB graphs with vertices of degree 3 for $v \leq 28$, we have observed no violations of the graph positivity for $v < 14$ vertices. A single violation is observed for $v = 14$. For $v \geq 14$, as the number v of vertices increases, the frequency of violations decreases. No positivity violation occurs in all RBB graphs with vertices of degree greater than 3, up to $v = 20$. For $v = 22$ and degree 4 there are two violations. For $r-$regular graphs with $r > 4$ the absence of violations could be checked up to $v = 20$. Although we found no positivity violation for RBB graphs with vertex degree larger than 4 in the large sample studied, we can point out examples of positivity violation occurring for larger values of v, in some $r-$regular graphs with $r = 5, 6, 7, 8$, which were defined in Ref.[7]. We conjecture that, for RBB graphs of any degree *the frequency of positivity violations becomes vanishingly small as v becomes large.*

An interesting observation emerging from the systematic study of RBB graphs with $v \leq 28$ and degree 3, is that the average order of the automorphism group of the graphs not satisfying the graph-positivity property is larger by an order of magnitude than the average order of the automorphism group for all RBB graphs.

In addition to this systematic survey of RBB graphs, we have focused the attention on the class of square and hexagonal lattices with periodic boundary conditions, which are also RBB graphs. In the case of rectangular grids of sizes $N_x \times N_y$ with periodic boundary conditions, we examined the cases $N_x = N_y$ up to sizes $N_y = 12$. For $N_x \geq N_y$ we found positivity violations only for $N_y = 4$ and $N_x \geq 432$.

For periodic hexagonal lattices of sizes $N_x \times N_y$ in the brick-wall representation, positivity is valid when $N_x \geq N_y$, apart from the case $N_x = N_y = 4$, while violations occur for $N_x < N_y$. We have tested this class of grids up to the size 14×14.

This positivity property can also be studied for graphs which are not RBB. Since we originally proposed the positivity conjecture for infinite square lattices, it is natural to consider also rectangular grids with open boundary conditions. In the case of rectangular grids $N_x \times N_y$ with open boundary conditions, in the cases $N_x = N_y$ we considered up to the case $N_y = 19$; the graph positivity holds except for the case of $N_x \times 3$ graphs. We have also examined the case of rectangular grids $N_x \times N_y$ with boundary conditions periodic only in the y direction. Again, we found positivity violations only for narrow grids, as in the case of rectangular grids with periodic and with open boundary conditions.

We considered also several cubic grids of sizes $N_x \times N_y \times N_z$ with open boundary conditions, up to the $5 \times 5 \times 4$ case: no positivity violation was observed, apart from the $N_x \times 2 \times 2$ case, which is isomorphic to the $N_y = 4$ rectangular grid case periodic in the y-direction.

In the case of non-bipartite graphs, the positivity property is not common. However there are exceptions for specific classes of graphs: for example, we have singled out a sequence of “nanotubes” C_{40+20N}, with N the number of hexagonal strips, and have tested graph positivity for $1 \leq N \leq 300$. All the nanotubes with $N > 7$ are graph-positive.

To perform our study of graphs, it was necessary to compute the graph matching generating polynomial

$$M(t) = \sum_{i=0}^{[v/2]} N(i) t^i \tag{1}$$

where $N(i)$ is the number of configurations of i dimers on the graph. We used the algorithm discussed in [8] to perform the computation.

The paper is organized as follows. In the second Section, we formulate the graph positivity property. The third Section summarizes the results of the graph tests for a variety of graphs and lattices. The fourth Section contains our conclusions. In Appendix A, the graph positivity is proven for polygons, for complete bipartite graphs and for an approximate average distribution of graphs. In Appendix B the positivity property is examined for a sequence of nanotubes.

II. THE POSITIVITY PROPERTY FOR GRAPHS

To formulate the graph-positivity properly, let us turn now to a cubic lattice graph G with v vertices of degree $2d$, and let $N(i)$ be the number of ways of setting down i dimers on the edges of G (with no overlap). If we consider the sequence of larger and larger periodic lattices used to compute the entropy $\lambda_d(p)$ on the infinite lattice, one must have

$$\hat{\lambda_d}(\hat{p_i}) = \frac{1}{v}\ln N(i) \rightarrow \lim_{v\to\infty} \frac{1}{v}\ln(\exp v\lambda_d) = \lambda_d(p) \tag{2}$$

where the arrow indicates convergence as $v \to \infty$. Here i is related to p by

$$\hat{p_i} = \frac{2i}{v} \approx p \tag{3}$$

where the integer i is chosen to make this approximation best. We refer now to the notation in Ref.[2] observing from Eq.(5.9) of this Ref. that

$$\lambda_d(p) = \frac{p}{2}\ln(2d) + \lim_{v\to\infty} \frac{1}{v}\ln Z \tag{4}$$

Observe now that Z can be factored into a “mean field” term Z_0 times the rest Z^* as in Eq.(5.12) of Ref.[2]

$$\lambda_d(p) = \frac{p}{2}\ln(2d) + \lim_{v\to\infty} \frac{1}{v}\ln(Z_0) + \lim_{v\to\infty} \frac{1}{v}\ln(Z^*). \tag{5}$$

From Eq.(2) and from Eq.(5.11) and (7.1) of Ref.[2], we have

$$\frac{1}{v}\ln(\frac{N(i)}{(2d)^i}) - \lim_{v\to\infty}\frac{1}{v}\ln(Z_0) \to \sum_{k=2} a_k(d)p^k \tag{6}$$

with

$$\lim_{v\to\infty}\frac{1}{v}\ln(Z_0) = -\frac{p}{2}\ln(p) - (1-p)\ln(1-p) - \frac{p}{2}. \tag{7}$$

It is an easy computation to show that for the graph $\bar{G}$, defined as the completion of G (namely the non-bipartite graph constructed by connecting the vertices of G in all possible ways), if we set $\bar{N}(i)$ as the number of ways of setting down i dimers on $\bar{G}$ (without overlap),

$$\bar{N}(i) = \frac{v!}{(v-2i)!i!2^i} \tag{8}$$

then

$$\frac{1}{v}\ln\frac{\bar{N}(i)}{(v-1)^i} \to \lim_{v\to\infty}\frac{1}{v}\ln(Z_0) \tag{9}$$

in the limit as $v \to \infty$ and with i chosen as before in Eq.(3). If one studies the definition of Z_0 in Ref.[2], the expression on the lhs of (9) is seen to arise naturally. But we get no theoretical understanding of why the completion of a graph, rather than the bipartite completion, is taken. Indeed, one could have in (9) used a similar expression with the bipartite completion, but one would have then ended with a less fruitful definition of graph positivity. We now define

$$d(i) \equiv \ln\frac{N(i)}{(2d)^i} - \ln\frac{\bar{N}(i)}{(v-1)^i} \tag{10}$$

and see that

$$\frac{1}{v}d(i) \to \sum_{k=2} a_k(d)p^k \tag{11}$$

The rhs of Eq.(11) is the series part of the dimer entropy in Eq.(6) in [4], where it is conjectured that the a_k are all positive. We now observe that as $v \to \infty$, the finite difference derivatives at $i = 0$ on the lhs of Eq. (11) become the derivatives on the rhs.

We write Δ for the finite difference derivative with respect to i. One has

$$\frac{v}{2}\Delta \approx \frac{d}{dp} \tag{12}$$

so differentiating Eq.(11) once, one gets

$$\frac{1}{2}(d(i+1) - d(i)) \to \frac{d}{dp}\sum_{k=2} a_k(d)p^k. \tag{13}$$

Writing $d(i) = \hat{d}(\hat{p})$ with $\hat{p} = \frac{2i}{v}$ and $h = \frac{2}{v}$, one has the Newton expansion

$$\hat{d}(\hat{p}) = \sum_{k=0}^{v/2} \frac{\Delta_h^k[\hat{d}](0)}{k!}(\hat{p})_k \tag{14}$$

where $(\hat{p})_k = \hat{p}(\hat{p}-h)...(\hat{p}-(k-1)h) = (\frac{2}{v})^k(i)_k$, $(i)_k$ is the falling factorial and Δ_h is the finite difference with step h, $\Delta_h\hat{d}(\hat{p}) = \frac{\hat{d}(\hat{p}+h)-\hat{d}(\hat{p})}{h}$.

We can now state the definition of graph positivity in greater generality. Let G be a simple regular connected bipartite (hence "biconnected") graph (RBB graph), with degree q and with v vertices. Let $\bar{G}$ be the completion (not the bipartite completion) of G. Let $N(i)$ be the number of ways of laying down i dimers on G (without overlap) and $\bar{N}(i)$ the same quantity for $\bar{G}$. Define

$$\hat{d}(\hat{p}) = d(i) = \ln\frac{N(i)}{q^i} - \ln\frac{\bar{N}(i)}{(v-1)^i}. \tag{15}$$

and

$$\hat{\lambda}(\hat{p}_i) = R(i) + \frac{h}{2}\sum_{k=0}^{v/2} \frac{\Delta_h^k[\hat{d}](0)}{k!}(\hat{p})_k \tag{16}$$

where

$$R(i) = \frac{1}{v}\ln(\frac{q^i}{(v-1)^i}\bar{N}(i)) \tag{17}$$

Using the Stirling formula for large v

$$R(i) \approx \frac{1}{2}(p\ln(q) - p\ln(p) - 2(1-p)\ln(1-p) - p) \tag{18}$$

Then G satisfies graph positivity, if all the $d(i)$ are non-negative, as are all terms derived by any number of non-trivial finite difference derivatives i.e. if all terms in the sequence $d(0), d(1), d(2), d(3), ...$ are non-negative as are all terms in the sequence $d(1) - d(0), d(2) - d(1), d(3) - d(2), ...$, and the sequence $d(2) - 2d(1) + d(0), d(3) - 2d(2) + d(1), d(4) - 2d(3) + d(2), ...$ etc. In fact, it is sufficient that the first term $\Delta^k d(0)$ in each of these sequences is non-negative, non-negativity of the other terms would then follow ($\Delta^k d(0) = 0$ for $k = 0, 1$ since $d(0) = d(1) = 0$). Equivalently, positivity means that all the coefficients in the Newton series of $\hat{d}(\hat{p})$ are non-negative.

It is natural to consider the series Eq.(16) also in the case of non-bipartite regular graphs.

Notice that using $N(1) = \frac{vq}{2}$ one can rewrite $d(i)$ in Eq.(15) with no explicit dependence on degree of the vertices

$$d(i) = \ln(\frac{N(i)}{N(1)^i}) - \ln(\frac{\bar{N}(i)}{\bar{N}(1)^i}) \tag{19}$$

for $i = 1, .., r$, where r is the maximum value of i with $N(i)$ not zero, and $\bar{N}(i)$ is the number of dimers on a complete graph with $\bar{v} = 2r$ vertices (if $\bar{v} = v$ the graph has perfect matchings). This suggests that it is worthwhile to investigate also when the graph-positivity holds for non-regular graphs or non-bipartite graphs.

III. TESTS OF GRAPH POSITIVITY

As a first step, we have tested systematically the validity of the positivity property on RBB graphs, exploring them in ascending number of vertices, namely we have counted the configurations of i dimers on these graphs and checked the inequalites for the higher finite differences. To generate systematically the RBB graphs, we have used the *geng* program in the *Nauty* package[5], via the *Sage* interface[6].

The first result of this extensive graph survey is that, while most RBB graphs share the graph-positivity property, a few of them do not, see Table I for the graphs with degree 3. There are no violations for $v < 14$.

to be changed: For $v = 30$ and degree 3 Nauty did not finish enumerating the graphs in ... days. Among the 23466000 graphs produced, there are 3948 violations.

For 3-regular graphs, the frequency of violations decreases with v, for $v \geq 14$.

It is interesting to observe that, in the cases considered in Table I, the average order of the automorphism group of the positivity-violating graphs is roughly an order of magnitude greater than the average order of the automorphism group of all the RBB graphs with the same degree, and that the ratio between these two numbers increases with v. In particular, the positivity violating graph with $v = 14$ is the most symmetrical of all $v = 14$ RBB graphs with degree 3.

For degrees greater than 3, there is no violation of positivity for RBB graphs with number of vertices up to $v = 20$. For $v = 22$, there are 2806490 RBB graphs with vertices of degree 4, and two violations. The average order of the automorphism group of the positivity-violating graphs is 1080., the average order of the automorphism group of all the RBB graphs with $v = 22$ and degree equal to 4 is 1.5.

TABLE I: For RBB graphs with $14 \leq v \leq 28$ vertices of degree 3, we have listed the number of graphs in this class, the number of violations of the graph positivity, the average order of the automorphism group of graphs ng, the average order of this group ngv for graphs violating the positivity property.

v	number of graphs	violations	ng	ngv
14	13	1	44.5	336.
16	38	2	18.6	112.
18	149	2	15.1	176.
20	703	8	8.7	118.
22	4132	17	4.5	72.
24	29579	49	3.3	92.
26	245627	115	2.3	66.
28	2291589	514	1.9	55.

Although in this systematic examination of graphs with low order we found no positivity-violating graphs with degree greater than 4, we can exhibit cases of positivity-violating graphs with degree up to 8, belonging to the class of k-regular graphs $G_{k,f}$ considered in Example 1 of Ref.[7]. The $G_{k,f}$ graphs, with $f \geq 2$ and $k \geq 3$ are RBB graphs with degree k and $v = 2n$ vertices where $n = (k^2 f + 1)$. The vertex classes of $G_{k,f}$ are

$$U = \{s\} \cup \{u_{a,b,c} : 1 \leq a \leq k; 1 \leq b \leq k; 1 \leq c \leq f\} \tag{20}$$

and

$$V = \{t\} \cup \{v_{a,b,c} : 1 \leq a \leq k; 1 \leq b \leq k; 1 \leq c \leq f\} \tag{21}$$

The edges are $E = E_1 \cup E_2 \cup E_3$ with

$$\begin{aligned} E_1 &= \{(u_{a,b,c}, v_{a,\beta,c}) : 1 \leq a, b, \beta \leq k; (b, \beta) \neq (1,1); 1 \leq c \leq f\} \\ E_2 &= \{(u_{a,1,c}, v_{a,1,c+1}) : 1 \leq a \leq k; 1 \leq c \leq f-1\} \\ E_3 &= \{(s, v_{a,1,1}) : 1 \leq a \leq k\}) \cup \{(u_{a,1,f}, t) : 1 \leq a \leq k\} \end{aligned} \tag{22}$$

and dimer countings for almost complete and complete matching

$$
\begin{aligned}
N(n-1) = \frac{((k-1)!)^{kf}}{(k-2)^2}&((k+2)^2(k-1)^{kf+2} + \\
&((k-2)^2 kf - 3k^2 + 4)k^2(k-1)^{(k-1)f} + \\
&2k^3(k-1)^{(k-2)f+1})
\end{aligned}
\tag{23}
$$

$$
N(n) = k((k-1)!)^{kf}(k-1)^{(k-1)f} \tag{24}
$$

The graph $G_{5,2}$ with 102 vertices of degree 5 and the graph $G_{6,2}$ with 146 vertices of degree 6 show a first violation in the case of $\Delta^2 d(i)$ for some $i > 0$. In the derivatives at $i = 0$, a first violation occurs for $\Delta^{13} d(0)$. The graphs $G_{7,2}$ and $G_{8,2}$ have $\Delta^{12} d(0) < 0$. The symmetry groups of the graphs $G_{k,2}$ with $k = 5, .., 8$ are larger than 10^{29}.

While all the examples of violations $\Delta^j d(i) < 0$ mentioned so far have $j \geq 2$, there are violations for $j = 1$. $\Delta d(i) \geq 0$ is equivalent to

$$
\frac{N(i)}{N(i+1)} \leq \frac{(2n-1)(i+1)}{r(n-i)(2n-2i-1)} \tag{25}
$$

where $v = 2n$ and r is the degree. This implies $N(n-1)/N(n) \leq n(2n-1)/r$. From Eqs.(23, 24) it follows that the graph $G_{3,6}$ with 110 vertices fails to satisfy this inequality.

The 0th order inequality $d(i) \geq 0$ gives

$$
N(i) \geq \frac{v! r^i}{(v-2i)! 2^i i! (v-1)^i} \tag{26}
$$

where r is the degree of the vertices. This inequality should be compared to the "Lower Matching Conjecture"[10]

$$
N(i) \geq \binom{n}{i}^2 (\frac{nr-i}{nr})^{nr-i} (\frac{ir}{n})^i. \tag{27}
$$

recently proven in [11]. In fact Csikvari proves a stronger bound with the right side of (27) divided by $\binom{n}{i}(i/n)^i(1-i/n)^{(n-i)}$. Preliminary numerical study suggests this new inequality supports the truth of (26). Gurvits has proved the following slightly weaker lower bound, see Eq.(51) of [12].

$$
N(i) \geq \frac{((r-i/n)/r)^{nr-i})(1-1/n)^{(1-1/n)(2n^2)(1-i/n)}}{((i/(nr))^i) n^{-2n(1-i/n)}((n(1-i/n))!)^2}
$$

We do not know whether there are violations of the inequality Eq.(26).

Let us now consider the case of a sequence of increasingly larger finite rectangular lattices with b.c. periodic in the x and y directions, as are used in the limiting procedure to extract

$\lambda_d(p)$ for $d = 2$. For this class of graphs, we have found no violation of graph-positivity for grids of sizes $(N_x \times N_y)$, with N_x even, such that

$4 \leq N_x \leq 430, N_y = 4$

$6 \leq N_x \leq 800, N_y = 6$

$8 \leq N_x \leq 100, N_y = 8$

and for the grids of sizes $N_x \times N_y = 10 \times 10, 12 \times 10, 12 \times 12$.

However the graphs are all not positive for

$430 < N_x \leq 5000, N_y = 4$.

We have examined also the hexagonal lattices of size $N_x \times N_y$ in the brick-wall representation. We have examined the following cases with $N_x \leq N_y$, with N_x even,

$4 \leq N_x \leq 800, N_y = 4$

$6 \leq N_x \leq 270, N_y = 6$

$8 \leq N_x \leq 90, N_y = 8$

$10 \leq N_x \leq 14, N_y = 10$

and $(N_x, N_y) = (12, 12), (14, 12), (14, 14)$. The only violation occurs in the case $(N_x, N_y) = (4, 4)$, which represents one of the two non positive 3-regular RBB graphs with 16 vertices.

For $N_x < N_y$, we have considered the cases

$N_x = 4, 6 \leq N_y \leq 100$, with all the graphs non positive.

$N_x = 6, 8 \leq N_y \leq 100$, with all the graphs $N_y \geq 26$ non positive.

The lattice 4×6, a graph with 24 vertices, is one of the 49 cases of violations observed in the systematic survey of the 3-regular RBB graphs with 24 vertices.

Let us now consider what happens in the case of non-RBB graphs, as mentioned at the end of Section II. In the case of disconnected graphs, the matching generating polynomial is the product of the matching generating polynomials of the connected components. Many violations of the graph positivity property are observed. For instance, the graph formed by n hexagons, with $n \leq 100$, violates positivity for $n \geq 3$.

For non-regular bipartite biconnected graphs there are in general many violations; for instance enumerating the bipartite biconnected graphs with minimum vertex degree 2 and maximum degree 3, the frequency of violations increases with v for $v = 10, ..., 18$.

Bipartite biconnected graphs with minimum degree 3 and maximum degree 4 have a similar pattern as RBB graphs, see Table II: the frequency of violations decreases with v

and, on the average, the non-positive graphs have significanty larger symmetries.

TABLE II: For connected bipartite graphs with v vertices of degree 3 or 4, we have listed the number of graphs, the number of violations of the graph positivity, the average order of the automorphism group of graphs ng, the average order of this group ngv for graphs violating the positivity property.

v	number of graphs	violations	ng	ngv
12	240	1	14.1	192.
14	5183	10	4.3	143.
16	190378	134	2.1	41.6
18	9816658	6291	1.5	14.8

Let us now consider some non-regular bipartite lattice graphs. In the case of rectangular grids of size $N_x \times N_y$, we found few violations, occurring in the case of narrow grids.

In the case of rectangular grids with b.c. periodic only in the y direction, we considered the cases in table III;

TABLE III: Sizes of the rectangular grids with b.c. periodic only in the y direction tested. We have tested the positivity of the grids for all values of N_x in the range indicated in the first row.

N_x	2-5600	2-2500	2-1500	2-1000	2-300	2-120	2-50	2-23
N_y	4	6	8	10	12	14	16	18

The only positivity violations found occur for $N_x \geq 421, N_y = 4$ and $N_x = 3, N_y = 18$.

In the case of rectangular grids with open boundary conditions we have considered the cases listed in the table IV.

We have found positivity violations only for $N_y = 3$.

Summarizing, in the case of rectangular grids with any boundary conditions, we have found no positivity violations for $N_y > 4$, y being the shortest direction.

In the case of cubic grids of sizes $N_x \times N_y \times N_z$ with open b.c., we have tested the positivity in the cases listed in the table V; there are no positivity violations except in the case $N_x \geq 421, N_y = 2, N_z = 2$ which is isomorphic to the rectangular grid $N_x \times 4$ periodic in the y-direction considered in table III.

As a final comment concerning biconnected non-bipartite graphs, it appears that the majority of these graphs do not have the graph-positivity property. We have checked that

TABLE IV: Tested rectangular grids $N_x \times N_y$ with open boundary conditions.

$N_x \leq 5000, N_y = 2$	$N_x \leq 500, N_y = 11$
$N_x \leq 1800, N_y = 3$	$N_x \leq 500, N_y = 12$
$N_x \leq 3700, N_y = 4$	$N_x \leq 180, N_y = 13$
$N_x \leq 3800, N_y = 5$	$N_x \leq 100, N_y = 14$
$N_x \leq 2700, N_y = 6$	$N_x \leq 70, N_y = 15$
$N_x \leq 2700, N_y = 7$	$N_x \leq 45, N_y = 16$
$N_x \leq 1700, N_y = 8$	$N_x \leq 50, N_x = 17$
$N_x \leq 1400, N_y = 9$	$N_x \leq 35, N_y = 18$
$N_x \leq 700, N_y = 10$	$N_x \leq 23, N_y = 19$

TABLE V: Sizes of the cubic grids tested. We have tested the positivity of the grids for all values of N_x in the range indicated in the first row.

N_x	2-5600	3-3500	4-2000	5-800	3-1600	4-500	5-150	4-85	5-13
N_y	2	3	4	5	3	4	5	4	5
N_z	2	2	2	2	3	3	3	4	4

this this is true for even v, $v \leq 8$. For odd v, $v \leq 9$ the frequency of violations increases fast and it is roughly 1/3 for $v = 9$. This is in agreement with the fact that infinite non-bipartite lattices have been found to be not graph-positive.

It would be interesting to investigate whether graphs which are not bipartite due to a few defects have the tendency to be positive.

We have examined the positivity of a sequence of nanotubes, C_{40+20N} in Appendix B for $1 \leq N \leq 300$. All these graphs are positive for $N > 7$. These graphs are formed by a nanotube composed of hexagons, and by two caps containing 6 pentagons each, and some more hexagons. Roughly speaking, the nanotube's hexagon lattice tube tends to make the graph positive, the pentagons negative, so if the nanotube is sufficiently long, one can expect the graph to be positive. However it does not seem to be generally true that a graph formed by a subgraph which is positive and a small non-bipartite part is positive. For instance consider a (N_x, N_y) rectangular grid with open boundary conditions, with $N_y = 5$. We saw that these graphs are positive (checked up to $N_y = 3800$). Let us create defects in the third and fourth vertical strip, by adding $SW-NE$ diagonals to its squares. We have considered these graphs up to $N_x = 4000$: for $N_x \geq 10$, all these graphs violate positivity.

IV. CONCLUSIONS

In a previous paper[4] we noticed that the dimer entropy of infinite bipartite lattices seem to satisfy a positivity property. We have shown that this positivity property can be generalized to finite graphs, as the positivity of the coefficients of the Newton expansion for the "dimer entropy" of graphs.

We considered two natural classes of finite graphs related to infinite bipartite lattices: the connected regular bipartite (RBB) graphs and finite lattices with various boundary conditions.

In the first class, we have tested exhaustively a very large sample of RBB graphs. The results of our survey lead us to conjecture that for all degrees r in $r-$regular graphs, the frequency of the positivity violations tends to zero as $v \to \infty$. Finally, we have also observed that the graphs showing positivity violations have an average order of the symmetry of the automorphism group sizably larger than the average order for graphs with the same number of vertices.

In the second class, we have examined a large number of rectangular grids $N_x \times N_y$ with various boundary conditions. We found no positivity violation for $min(N_x, N_y) > 4$.

In the three-dimensional case we could only verify the positivity for relatively small cubic grids (with open b.c.). These results give some support to the conjecture that for the infinite hypercubic lattices in any dimension, with open b.c., all the coefficients of the series for the dimer entropy are positive[4].

In the case of hexagonal lattices, in the brick-wall representation $N_x \times N_y$, we found no violations for $N_x \geq N_y$, except for $N_x = N_y = 4$, while there are several violations for $N_x < N_y$. This may be related to the fact that the entropy of the hexagonal lattice depends on the b.c.[14]. Also in this case these computations suggest that when taking the limit $N \to \infty$ for the $N \times N$ cases, the coefficients of the Newton expansion for the dimer entropy of the infinite hexagonal lattice are all positive.

V. APPENDIX A: PROOF THAT C_{2n} AND $K_{v,v}$ ARE GRAPH-POSITIVE

A polygon C_v with v vertices has $N(i) = \frac{v}{v-i}\binom{v-i}{i}$ [13]. From (19) one gets for v even

$$d(i) = \ln(\frac{(v-i-1)!(v-1)^i}{(v-1)!}) \tag{28}$$

from which

$$\Delta d(i) = -\ln(1 - \frac{i}{v-1}) = \sum_{j=1}^{\infty} \frac{i^j}{j(v-1)^j} \tag{29}$$

which is positive; and thus from $d(1) = 0$ one sees that $d(2), d(3), ...$ are positive.

$$\Delta^{(k+1)} d(i) = \sum_{j=1} \frac{\Delta^k (i^j)}{j(v-1)^j} \tag{30}$$

Observing that $i^j = \sum_{h=0}^{j} S_{j,h}(i)_h$, with $S_{j,h}$ Stirling numbers (of the second kind), and that $\Delta(i)_m = m(i)_{m-1}$, from the positivity of the Stirling numbers and of the falling factorials, it follows that $\Delta^k d(i)$ is positive for $k \geq 1$, so that C_v is graph-positive for v even.

A complete bipartite graph $K_{n,n}$ has $N(i) = \binom{n}{i}^2 i!$.

$$d(i) = \ln(\frac{n!}{(n-i)!(2n-1)(2n-3)...(2n-2i+1)}(\frac{2n-1}{n})^i) \tag{31}$$

One has

$$d(i+1) = d(i) + \ln(\frac{(n-i)(2n-1)}{(2n-2i-1)n}) = d(i) + \ln(1 + \frac{i}{(2n-2i-1)n}) > d(i) \tag{32}$$

for $i < n$; since $d(1) = 0$ it follows that $d(i) \geq 0$ for $i < n$. One has

$$\Delta d(i) = \ln(\frac{(2n-1)(n-i)}{n(2n-2i-1)}) = \ln(1 + \frac{i}{n(2n-2i-1)}) \tag{33}$$

so that $\Delta d(i) > 0$ for $i < n$. From

$$\Delta d(i) = \ln(\frac{2n-1}{2n}) - \ln(1 - \frac{1}{2(n-i)}) = \ln(\frac{2n-1}{2n}) + \sum_{j=1} \frac{1}{j2^j} \frac{1}{(n-i)^j} \tag{34}$$

it follows that for $m \geq 1$

$$\Delta^{m+1} d(i) = \sum_{j=1} \frac{1}{j2^j} \Delta^m (\frac{1}{(n-i)^j}) \tag{35}$$

defined for $i \leq n-m-1$. It is not difficult to show these are non-negative, observing that

$$\Delta \prod_j \frac{1}{(n-i-n_j)}$$

where $0 \leq n_j < k$, is the sum of terms of the form

$$\prod_j \frac{1}{(n - i - n'_j)}$$

where $0 \leq n'_j < k + 1$. Therefore $K_{n,n}$ is graph-positive.

Friedland, Krop and Markstom[16] have computed an approximation for the average value of $N(i)$ over all $0-1$ $n \times n$ matrices with row and column sums equal to r

$$N^{Av}(i) = \frac{\binom{n}{i}^2 r^{2i} i!(rn - i)!}{(rn)!} \tag{36}$$

One can show by the techniques of this section that the sequence of $N^{Av}(i)$ leads to $d(i)$ satisfying graph positivity. This is very consistent with our conjecture that as $n \to \infty$ the frequency of violations of graph positivity goes to zero.

VI. APPENDIX B: A SEQUENCE OF NANOTUBES

A fullerene can be drawn on a sphere; it has 12 pentagonal faces, while the other faces are hexagons.

A nanotube C_{40+20N} can be formed by cutting a C_{40} fullerene into a North cap and a South cap, joined by a tube formed by hexagons, belonging to an hexagon lattice, formed by N hexagonal strips with 20 nodes characterized by a "chiral vector" (m, n) which describes the periodicity conditions on the tube. In the case we have considered $m = n = 5$.

In the algorithm[8] for computing the matching generating polynomial, the ordering of the edges is important for performance.

TABLE VI: North cap

0-2	2-8	6-8	3-6	0-3	0-1	3-4	6-7
8-9	2-5	4-18	17-18	1-17	1-14	16-17	18-19
4-21	5-13	12-13	13-14	5-10	20-21	19-20	21-22
7-22	7-25	22-23	23-24	24-25	25-26	9-26	9-29
26-27	10-29	28-29	27-28	10-11	11-12	14-15	15-16

In Tables VI, VII, VIII the edges must be read in reading order, from left to right, from up to down. The edges are ordered in such a way that the maximum number of 'active nodes'[8] is 11.

FIG. 1: Nanotube with $N = 1$; if the letter a is present in a node index, add 20 to the node index.

We considered $1 \leq N \leq 300$; graph positivity holds for $N > 7$.

TABLE VII: Strips: the first index in an edge $a-b$ stands for $a+20i$ or for $a+20(i+1)$ if it is followed by an A; the second index b stands for $a+20(i+1)$; 20 is the number of nodes added by a strip; $i=0,...,N-1$ where N is the number of strips.

11-14	12-17	15-18	17A-18	16A-17
19-22	16-21	21A-22	20A-21	18A-19
19A-20	22A-23	20-25	23-26	25A-26
24A-25	23A-24	26A-27	24-29	27-10
10A-29	28A-29	27A-28	28-13	13A-14
10A-11	11A-12	12A-13	14A-15	15A-16

TABLE VIII: South cap; to the indices of the edges one must add $20N$

11-37	28-35	35-37	33-35	34-37
27-36	24-36	36-38	33-38	38-39
23-39	20-39	32-33	19-32	31-32
16-31	31-34	30-34	12-30	15-30

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