AN IMPROVED UPPER BOUND FOR THE
THREE DIMENSIONAL DIMER PROBLEM

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ABSTRACT. Let n be even and denote by $f(n)$ the number of domino tilings of a cube of side n. The three dimensional dimer problem is to determine the limit $\ell_3 := \lim_{n\to\infty}(\log f(n))/n^3$ (which is known to exist). The best previously known upper bound was found by Minc and is $1/12 \log 6! = 0.54827....$ In this paper we improve this bound to 0.463107.

1. Introduction

The dimer problem, which in dimension three is one of the classical unsolved problems in solid-state chemistry, is the following. Define an *brick* to be a d-dimensional ($d \geq 2$) rectangular parallelepiped with sides of integer lengths; we will always assume its volume to be even. A brick of volume 2 is called a *dimer*. The problem is to determine the number $f(a_1, \ldots, a_d)$ of dimer tilings of the brick with sides of lengths $a_1, \ldots, a_d$.

It is remarkable that for $d = 2$ this number can be expressed in closed form, as was shown independently by Fisher, Kasteleyn and Temperley (see [**14**] and [**6**]). In contrast, for $d \geq 3$ no such formulas are known. Moreover, the number of dimer tilings of a brick of dimension at least three is not known even asymptotically. More precisely, Hammersley proved [**4**] that the sequence $1/(a_1 \cdots a_d) \log f(a_1, \ldots, a_d)$ approaches a finite limit ℓ_d as $a_i \to \infty$, $i = 1, \ldots, d$. However, the exact value of ℓ_d is not known for $d \geq 3$. The most important case for applications is the case $d = 3$ [**5**][**7**].

Various upper and lower bounds for ℓ_3 have been proved starting as far back as six decades ago, when Fowler and Rushbrooke [**3**] showed (assuming, based on physical and heuristic arguments, that the limit defining ℓ_d exists) that

$$0 \leq \ell_3 \leq \frac{1}{2} \log 3 = 0.54931...$$

This upper bound was improved by Minc [**8**] to $1/12 \log 6! = 0.54827...$, which represents the best upper bound previously known.

On the other hand, since ℓ_d is clearly a nondecreasing function of d, one obtains that a lower bound for ℓ_3 is given by ℓ_2, which was determined by Fisher, Kasteleyn and Temperley to be

$$\ell_2 = 1/\pi \sum_{r \geq 0} (-1)^r / (2r+1)^2 = 0.29156...$$

This lower bound has been improved several times, first by Fisher [**1**] to 0.30187, then by Hammersley [**5**] to 0.418347 and finally by Priezzhev [**11**] to 0.419989. A conjecture due to Schrijver and Valiant on lower bounds for permanents* [**13**] would imply, as noted by Minc [**9**], that $\ell_3 \geq 0.440075$.

Nagle [**10**] obtained the heuristic estimate of 0.446 for the actual value of ℓ_3.

The main purpose of this paper is to prove the following result.

THEOREM1.1. $\ell_3 \leq 0.463107$.

Our proof employs the transfer matrix method to encode the dimer tilings of a (toroidal) brick as closed walks in a certain graph. Using the transfer matrix theorem we obtain a family of upper bounds for ℓ_3 expressed in terms of the largest eigenvalues of our graphs. The problem is then reduced to determining (or finding a good upper bound for) the largest eigenvalue of a certain nonnegative symmetric matrix of order 2^{16}. To this end, we take advantage of a certain group G of permutation matrices which commute with our matrix. It turns out that the eigenvalue we need to estimate is the same as the largest eigenvalue of the action of our matrix on the subspace of G-invariants. This is given by a sparse nonnegative matrix A of order 222. Finally, we use an elementary way to obtain upper bounds for the largest eigenvalue of A in terms of the trace of even powers of A. The bound in Theorem 1.1 is obtained by computing the 16-th power of A. We also show that knowledge of the exact value of the largest eigenvalue of A could improve the upper bound by at most lowering the last digit from 7 to 5.

From the above outline of our proof it might seem that the success of our approach is conditioned by the progress in computational power that occurred since the previous upper bounds have been found. However, it turns out that one can derive by our method the already improved upper bound of 0.519093, and the largest computation involved in the process is finding the trace of the fourth power of a sparse matrix of order 22.

Our approach to this problem seems not to have been considered before. In contrast to Minc's method, which used a general inequality for permanents to deduce an upper bound for ℓ_3, our setup allows one to take advantage of the specific problem at hand. It is probably this fact that accounts for the significant improvement in the upper bound.

2. A family of upper bounds

Let $f_t(k,l,n)$ be the number of dimer tilings of the *toroidal* brick $T(k,l,n)$ of sides k, l and n. Clearly, $f(k,l,n) \leq f_t(k,l,n)$, and therefore

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*Recently, Schrijver has proved this conjecture (see A. Schrijver, "Counting 1-factors in regular bipartite graphs," *J. Combin. Theory Ser. B,* **72** (1998), 122–135).

$$\ell_3 \le \lim_{n\to\infty} \frac{1}{n^3} \log f_t(n) \tag{2.1}$$

(here $f_t(n)$ stands for $f_t(n,n,n)$, and n is even). In fact, it follows from the results in [**4**] that equality holds in (2.1), but this will not be needed in our proof.

Define a weighted directed graph S as follows. Take the set of vertices of S to be the set of k by l 0-1 matrices. For two such matrices s and t, define the weight of the edge from s to t to be zero unless the supports of s and t are disjoint. If the supports are disjoint, consider a $k \times l$ toroidal brick (i.e., a toroidal chessboard) and remove from it the unit squares corresponding to nonzero entries of s and t; define the weight of the edge from s to t to be the number of dimer coverings of the leftover part.

Let $\lambda_{k\times l}^{(i)}$, $i = 1, \ldots, 2^{kl}$, be the eigenvalues of the adjacency matrix M of S. Since this is a nonnegative matrix, by the Perron-Frobenius theorem its largest eigenvalue is real and positive. Denote it by $\lambda_{k\times l}$. Note also that it follows from the definition that M is symmetric, and hence all its eigenvalues are real.

PROPOSITION 2.1.
$$f_t(k,l,n) = \sum_{i=1}^{2^{kl}} \left(\lambda_{k\times l}^{(i)} \right)^n.$$

Proof. Let $\mathcal{T}$ be a dimer tiling of the toroidal brick $T(k,l,n)$. Regard our brick as a stack of n horizontal layers, each consisting of a $k \times l$ toroidal array of unit cubes. In each such layer, write 1's in the unit cubes covered by a dimer extending into the next layer above (for the top layer, dimers extending into the bottom layer); write zeroes in the remaining unit cubes. In this way, our tiling is associated a closed walk C on n steps in the graph S. By the definition of S, the weight of C (i.e., the product of the weights of its steps) is equal to the number of tilings of $T(k,l,n)$ whose associated closed walk is C.

Therefore, $f_t(k,l,n)$ is just the total weight of closed walks on n steps in S (if $e_1 e_2 \cdots e_n$ is a closed walk, then $e_i e_{i+1} \cdots e_n e_1 \cdots e_{i-1}$ is in general a different closed walk). Since by the transfer matrix theorem (see e.g. [**12**]) this is just the trace of M^n, the statement of the Proposition follows. $\square$

LEMMA 2.2. *If l and n are even, we have*

$$\frac{1}{kn} \log \lambda_{k\times n} \le \frac{1}{n} \log 2 + \frac{1}{kl} \log \lambda_{k\times l}.$$

Proof. Since all eigenvalues are real and l and n are even, we obtain using Proposition 2.1 that

3

$$\left(\lambda_{k\times n}\right)^l \leq \sum_{i=1}^{2^{kn}} \left(\lambda_{k\times n}^{(i)}\right)^l$$
$$= f_t(k, n, l)$$
$$= f_t(k, l, n)$$
$$= \sum_{i=1}^{2^{kl}} \left(\lambda_{k\times l}^{(i)}\right)^n$$
$$\leq 2^{kl} \left(\lambda_{k\times l}\right)^n .$$

The desired inequality follows by taking the logarithms of the extreme terms above and dividing through by kln. $\square$

PROPOSITION 2.3. *For even k and l, we have*

$$\ell_3 \leq \frac{1}{kl} \log \lambda_{k\times l}.$$

Proof. Let n be even and set $k = l = n$ in Proposition 2.1. Since all the eigenvalues are real, we obtain

$$f_t(n) = \sum_{i=1}^{2^{n^2}} \left(\lambda_{n\times n}^{(i)}\right)^n \leq 2^{n^2} \left(\lambda_{n\times n}\right)^n .$$

Taking the logarithm on both sides and dividing through by n^3 we deduce

$$\frac{1}{n^3} \log f_t(n) \leq \frac{1}{n} \log 2 + \frac{1}{n^2} \log \lambda_{n\times n}. \tag{2.2}$$

Setting $l = k, k = n$ in Lemma 2.2 one obtains

$$\frac{1}{n^2} \log \lambda_{n\times n} \leq \frac{1}{n} \log 2 + \frac{1}{kn} \log \lambda_{k\times n}. \tag{2.3}$$

By (2.2), (2.3) and Lemma 2.2 it follows that

$$\frac{1}{n^3} \log f_t(n) \leq \frac{1}{n} \log 2 + \frac{1}{n^2} \log \lambda_{n\times n}$$
$$\leq \frac{2}{n} \log 2 + \frac{1}{kn} \log \lambda_{k\times n}$$
$$\leq \frac{3}{n} \log 2 + \frac{1}{kl} \log \lambda_{k\times l}.$$

Since this is true for all even n, the statement of the Proposition follows from (2.1). $\square$

4

REMARK 2.4. In fact, the arguments in [**2**] imply that

$$\lim_{n\to\infty} \frac{1}{n^3} f_t(n) = \lim_{n\to\infty} \frac{1}{kl} \log \lambda_{k\times l}.$$

Therefore, since by [**4**] equality holds in (2.1), we obtain that ℓ_3 is the limit of the upper bounds of Proposition 2.3, as $k, l \to \infty$.

One can expect, in view of Remark 2.4, that as the values of k and l in Proposition 2.3 increase, the upper bounds get closer to the actual value of ℓ_3. For $k = 2$, $l = 4$ we obtain the already improved bound of 0.518971 (it is interesting that the slightly weaker bound of 0.519093 can be obtained without using the computer; see Section 5). For $k = 2$, $l = 6$, only the relatively small improvement to 0.513456 is obtained. However, $k = l = 4$ yields the bound in Theorem 1.1.

3. Estimation of $\lambda_{4\times4}$

Consider the graph S defined in the previous section. Denote its incidence matrix by M.

Let s and t be two vertices of S (i.e., two k by l matrices with entries 0 or 1) and suppose the (s, t) entry of M is nonzero. By the definition of S, this means that the supports of s and t are disjoint, and moreover, the board obtained from a k by l toroidal chessboard by removing the squares corresponding to the nonzero entries of s and t has at least one dimer covering. This clearly implies that the numbers of 1's in s and t have the same parity. Therefore, M is the direct sum of the incidence matrix of the subgraph of S consisting of vertices with an even number of 1's and the incidence matrix corresponding to vertices with an odd number of 1's; denote these two matrices by A and B, respectively.

Let $\mathcal{F}$ be the set of vertices of S involving an even number of 1's. Regard A as a linear transformation on the vector space V with basis $\mathcal{F}$.

Let G be a group of symmetries of a k by l toroidal chessboard. The group G acts in a natural way by permutations on $\mathcal{F}$. Extend this linearly to an action on V.

LEMMA 3.1. *The matrix A commutes with the action of G on V.*

Proof. It suffices to check that for each vector $s \in \mathcal{F}$ we have $g \cdot A(s) = A(g \cdot s)$, for all $g \in G$. This follows from the fact that g is a symmetry of the toroidal board. $\square$

The following result is quite possibly known, but we were not able to find it in the literature.

LEMMA 3.2. *If N is a nonnegative matrix that commutes with a group of permutation matrices G, then the largest eigenvalue of N is the same as the largest eigenvalue of N acting on the subspace of G-invariants.*

The elegant argument given below is due to Phil Hanlon. Our original formulation of Lemma 3.2 assumed that G is abelian, and the proof used character theory (this weaker version suffices to prove Theorem 1.1, but a considerable amount of computational time can be saved using the stronger version).

5

Proof. By the Perron-Frobenius theorem we know that the eigenvalue λ of largest absolute value is real and positive, and among the eigenvectors of this eigenvalue there is one with nonnegative coordinates; denote it by v. Define

$$v_0 = \frac{1}{|G|} \sum_{g \in G} g \cdot v. \tag{3.1}$$

Since N commutes with G, v_0 is also an eigenvalue for λ, and it is clear that v_0 is G-invariant. Moreover, since the coordinates of $g \cdot v$ are a permutation of the coordinates of v, it follows from (3.1) that for any coordinate of v that is strictly positive, the corresponding coordinate of v_0 is also strictly positive, so in particular v_0 is nonzero. $\square$

Let $O_1, O_2, \ldots, O_p$ be the orbits of the action of G on $\mathcal{F}$. For $1 \le i \le p$ define

$$v_i = \frac{1}{|G|} \sum_{g \in G} g \cdot e_i,$$

where e_i is some fixed element of O_i, $i = 1, \ldots, p$. Since the subspace V^G of G-invariants is the image of the projection $\phi : V \to V$, $\phi = (1/|G|) \sum_{g \in G} g$, the vectors v_i form a basis for V^G. Since by Lemma 3.1 A commutes with G, V^G is invariant under A. The matrix of the restriction of A to V^G is given by

$$\begin{aligned}
Av_i &= \frac{1}{|G|} A \left(\sum_{g \in G} g \cdot e_i \right) \\
&= \frac{1}{|G|} \sum_{g \in G} g \cdot Ae_i \\
&= \frac{1}{|G|} \sum_{g \in G} g \cdot \left(\sum_{m=1}^{n} a_{im} e_m \right) \\
&= \sum_{m=1}^{n} a_{im} \frac{1}{|G|} \sum_{g \in G} g \cdot e_m \\
&= \sum_{j=1}^{p} \left(\sum_{m \in O_j} a_{im} \right) v_j, \tag{3.2}
\end{aligned}$$

where n is the order of the matrix A.

Therefore, by Lemma 3.2, in order to estimate the largest eigenvalue of A it suffices to estimate the largest eigenvalue of the matrix A^G whose (i, j) entry equals $\sum_m a_{im}$, the sum running over the elements of the orbit O_j.

Let $k = l = 4$. It is easy to see that there exists a group of symmetries of the 4×4 toroidal chessboard isomorphic to the semidirect product of $C_4 \times C_4$ with D_8, where C_4

6

is the cyclic group of order 4 and D_8 is the dihedral group of order 8 (the three factors correspond to shifting the toroidal board vertically and horizontally, and to the symmetry group of a square).

However, the full symmetry group is in fact three times larger than this. Indeed, the 4×4 toroidal chessboard is, quite remarkably, isomorphic to the four-dimensional hypercube (this useful observation is due to the referee). Therefore, its symmetry group is isomorphic to the semidirect product of $(C_2)^4$ with the symmetric group S_4 (the first four factors correspond to reflections across hyperplanes parallel to the coordinate hyperplanes, while the last one corresponds to permuting the four coordinate axes). Choose G to be this group.

The family $\mathcal{F}$ consists of 2^{15} vectors. It turns out that the action of G on these vectors has 222 orbits, so the matrix A^G whose largest eigenvalue we need to estimate is of order 222. Exact calculation of the eigenvalues of a matrix of this size is beyond the capabilities of (at least most) present-day computers. To resolve this we employ the following simple result.

LEMMA 3.3. *Let C be a nonnegative matrix and let λ be its largest eigenvalue. If all eigenvalues of C are real, then for all $i \geq 1$ we have*
  (a) $\lambda \leq tr(C^{2i})^{1/2i}$
  (b) $\lambda^2 \geq tr(C^{2i+2})/tr(C^{2i})$.

Proof. Let $\lambda_1, \ldots, \lambda_q$ be the eigenvalues of C. Since they are real, we have

$$\mathrm{tr}(C^{2i}) = \sum_{j=1}^{q} (\lambda_j)^{2i} \geq \lambda^{2i}.$$

To obtain (b), notice that since λ is the largest eigenvalue, one has

$$\mathrm{tr}(C^{2i+2}) = \sum_{j=1}^{q} (\lambda_j)^{2i+2}$$
$$\leq \sum_{j=1}^{q} \lambda^2 (\lambda_j)^{2i}$$
$$= \lambda^2 \mathrm{tr}(C^{2i}).$$

$\square$

Since A^G is sparse, its powers can be found in a reasonable time using the computer (we are indebted to John Stembridge for writing an efficient program to this end). The traces of the first 16 powers of A^G were found in about 24 minutes of CPU time. The traces of the 14-th and 16-th powers are

$$t_{14} = 1126977601503291741399637139638752100045480750$$
$$t_{16} = 30751614759537810099863628179379072700939762213987550.$$

7

Applying Lemma 3.3 to A^G, we obtain that the largest eigenvalue λ_A of A satisfies

$$1651.87\cdots = \left(\frac{t_{16}}{t_{14}}\right)^{1/2} \leq \lambda_A \leq (t_{16})^{1/16} = 1651.93\ldots \tag{3.3}$$

The matrix B corresponding to the vertices of S with an odd number of 1's can be analized in a completely analogous way. Its G-invariant part B^G turns out to have order 181. The trace of the square of B^G is found with the computer to be

$$t_2' = 2199876.$$

Lemma 3.3(a) with $i = 1$ implies therefore that

$$\lambda_B \leq \sqrt{2199876} < 1484 < \lambda_A.$$

Thus $\lambda_{4\times 4} = \lambda_A$. Theorem 1.1 follows then from the upper bound in (3.3) and Proposition 2.3. From the lower bound in (3.3) it follows that $(1/16)\log\lambda_{4\times 4} > 0.463104$, and therefore the precise knowledge of $\lambda_{4\times 4}$ could bring only a very slight improvement on the bound from Theorem 1.1.

4. Higher dimensions and other dimer enumeration problems

The ideas in Section 2 can be generalized without difficulty to the case of a d-dimensional brick. The only limitation is that the number of vertices in the corresponding graph S_d increases very fast with d, and therefore the size of the matrices whose largest eigenvalues we need to estimate quickly go beyond the capabilities of (at least today's) computers. However, we do obtain an improvement on the upper bound for ℓ_4 at a very small expense of computation time (in fact, as we will discuss below, this could almost be worked out by hand). We also indicate how this bound could be improved further by performing a longer computer calculation. Finally, we point out another feasible computer calculation that would quite likely improve the best known upper bound for ℓ_5. However, since from the perspective of applications almost all attention seems to be concentrated on the three-dimensional case, we did not carry out these computations.

In analogy to Section 2, define the graph $S = S_d$ to have its vertex set consisting of $(d-1)$-dimensional arrays of 0's and 1's, the dimensions of the array being $a_1, \ldots, a_{d-1}$. Define the edge-weights of S in analogy to the definition in Section 2.

Let $\mathbf{a}$ denote the vector $(a_1, \ldots, a_{d-1})$. Let $\lambda_{\mathbf{a}}$ be the largest eigenvalue of the incidence matrix of S. The following result can be proved using arguments similar to the ones in Section 2.

PROPOSITION 4.1. *For even $a_1, \ldots, a_{d-1}$, we have*

$$\ell_d \leq \frac{1}{a_1 \cdots a_{d-1}} \log \lambda_{\mathbf{a}}.$$

Let $d=4$ and choose $a_1 = a_2 = a_3 = 2$. The incidence matrix M of S is again (as in Section 3) the direct sum of two sparse matrices A and B; both have order 128. Given

8

the manageable size, one can use the computer to find the first few powers of A and B, and then deduce by Lemma 3.3 a good upper bound for $\lambda_{2,2,2}$. Using Proposition 4.1, this yields

$$\ell_4 \leq 0.662561,$$

which is slightly better than the best previously known upper bound of $1/16 \log 8! = 0.662788...$, due to Minc [**8**]. (Note that if we exploit the fact that the natural action of the symmetry group of the cube commutes with A and B, the computation is reduced to the degree that it can almost be done by hand; see Section 5).

We note that the case $a_1 = a_2 = 2$, $a_3 = 4$ is also within reach: choosing G to be the symmetry group of the $2 \times 2 \times 4$ toroidal brick, the matrix A^G has order 1324. The case $d = 5$, $a_1 = a_2 = a_3 = a_4 = 2$ reduces to a calculation of smaller size.

Finally, we mention that our method also applies to other dimer enumeration problems in three (or higher) dimensions that should be of comparable interest, e.g. for toroidal quotients of the body centered cubic lattice or face centered cubic lattice. Indeed, these lattices satisfy the three crucial properties required for the ideas in Section 2 to go through: (1) if $g(a, b, c)$ is the number of dimer coverings of a toroidal quotient of sizes a, b and c then g is symmetric in a, b, c (2) the dimer coverings can be interpreted as closed walks in a certain weighted directed graph S and (3) the adjacency matrix of S is symmetric.

5. Concluding remarks

As promised, we argue in this section that the case $d = 3$, $k = 2$, $l = 4$ can be worked out with minimal (conceivably even no) computer assistance.

The matrix M has in this case order 2^8, so the direct summands A and B both have order 128. Figure 5.1 illustrates the vertices of the graph S which give rise to A. Each such vertex, by definition a 2 by 4 0-1 matrix (with an even number of 1's), is identified with a (toroidal) 2×4 chessboard whose unit squares corresponding to 1's in the matrix are shaded.

Choose G to be the group generated by the shift one unit to the right and by the reflection in the horizontal and vertical symmetry axes of the board (so G is isomorphic to $C_4 \times C_2 \times C_2$). The action of G on the vertices of A turns out to have the 22 orbits indicated in Figure 5.1.

By (3.2), the largest eigenvalue of A is the same as the largest eigenvalue of the matrix A^G of order 22 whose (i, j) entry is obtained as follows: choose some element x in the i-th orbit and add up the weights of the edges of S from x to y, as y runs over the j-th orbit.

This can be done by inspection from Figure 5.1. For example, let us find the $(6, 14)$ entry of our matrix A^G. To this end, let x be the top element of orbit 6. Only the second, third, sixth and seventh elements of orbit 14 have their shaded squares in positions disjoint from the positions of the shaded squares of x. Moreover, by superimposing x and any of these four elements of orbit 14, the unshaded part of the resulting (toroidal) board has always two distinct dimer coverings. Therefore, $A^G(6, 14) = 8$. Similarly, one obtains $A^G(6, 15) = 0$ and $A^G(6, 21) = 4$.
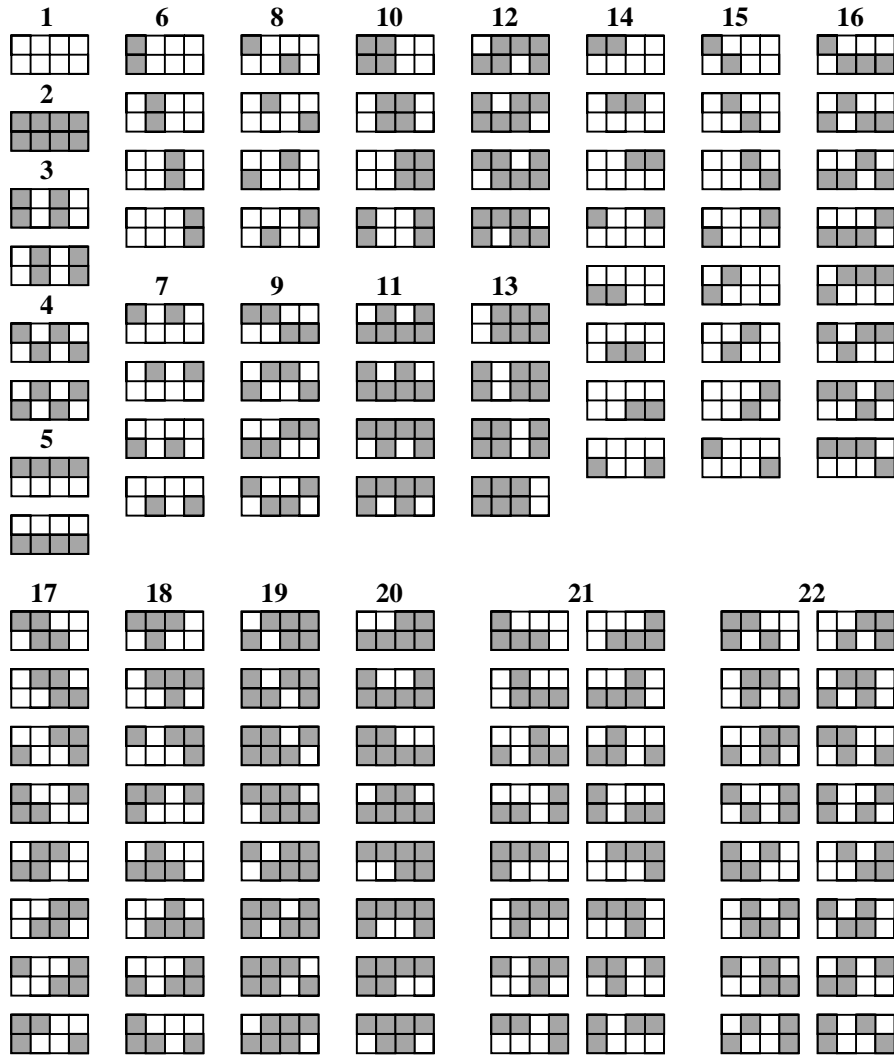
9

FIGURE 5.1

Most of the entries of A^G turn out to be zero. This makes it very easy to compute its square, and therefore the trace of its second and fourth powers. The values of these traces are

$$t_2 = 4462$$
$$t_4 = 16369814. \tag{5.1}$$

The matrix B can be handled in a completely analogous way. As in Section 3, it turns out that the largest eigenvalue of B is strictly less than the largest eigenvalue of A. Thus,

10

by (5.1) and Lemma 3.3 one obtains for ℓ_3 the upper bounds of 0.52521 (from t_2) and 0.519093 (from t_4).

We conclude with some comments on the case $k = 4$, $l = 6$. This would most likely improve on the upper bound in Theorem 1.1. However, unless one could find some additional reductions besides the ones discussed in Section 3, the size of the data one needs to handle surpasses the limits of today's computers. Indeed, the matrix A has in this case order 2^{23}, while the largest group G we can choose is the symmetry group of a 4 by 6 toroidal chessboard, which has 96 elements.

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