

*Discussiones Mathematicae*  
*Graph Theory* 33 (2013) 531–557  
doi:10.7151/dmgt.1707

## COUNTING MAXIMAL DISTANCE-INDEPENDENT SETS IN GRID GRAPHS

REINHARDT EULER

*Université Européenne de Bretagne and Lab-STICC, CNRS, UMR 6285,  
Université de Brest, B.P.809,  
20 Avenue Le Gorgeu, 29285 Brest Cedex, France*

**e-mail:** Reinhardt.Euler@univ-brest.fr

PAWEŁ OLESIK<sup>1</sup>

*AGH University of Science and Technology,  
Faculty of Geology, Geophysics and Environment Protection,  
Department of Geoinformatics and Applied Computer Science,  
30-059 Cracow, Poland*

**e-mail:** oleksik@agh.edu.pl

AND

ZDZISŁAW SKUPIEŃ

*AGH Kraków  
al. Mickiewicza 30, 30-059 Kraków, Poland*

**e-mail:** skupien@agh.edu.pl

### Abstract

Previous work on counting maximal independent sets for paths and certain 2-dimensional grids is extended in two directions: 3-dimensional grid graphs are included and, for some/any  $\ell \in \mathbb{N}$ , maximal distance- $\ell$  independent (or simply: maximal  $\ell$ -independent) sets are counted for some grids. The transfer matrix method has been adapted and successfully applied.

**Keywords:** independent set, grid graph, Fibonacci, Padovan numbers, transfer matrix method.

**2010 Mathematics Subject Classification:** 11B39, 11B83, 05A15, 05C69.

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<sup>1</sup>Work supported by the AGH-UST Fac. of GG&EP Research Plan, Task No. 11.11.140.032.

## 1. INTRODUCTION

Given natural numbers  $p, q, n$ , the symbol  $G_{p,q,n} = (V, E)$  stands for the 3-dimensional grid graph of size  $p \times q \times n$  (or  $(p, q, n)$ -grid graph) with vertex set

$$V = \{(i, j, k) : 1 \leq i \leq p, 1 \leq j \leq q, 1 \leq k \leq n\}$$

and edge set

$$E = \{(i, j, k), (i', j', k') : |i - i'| + |j - j'| + |k - k'| = 1\}.$$

A subgraph of a grid  $G$  (with fixed  $p$  and  $q$ ) induced by vertices with last component  $k$ , denoted by  $S_k$ , is called a *slice*  $k$  of  $G$ .

Given a graph  $G$  and an  $\ell \in \mathbb{N}$ , a set  $I$  of vertices of  $G$  is called  $\ell$ -*independent* in  $G$  if any shortest path between two elements of  $I$  has length at least  $\ell + 1$ , or equivalently, if on any path between two elements of  $I$  there are at least  $\ell$  vertices not belonging to  $I$ .

A maximal (with respect to set inclusion)  $\ell$ -independent set  $B$  in  $G = G_{p,q,n}$  is called an  $\ell$ -*basis* of  $G$ . We let  $B_{p,q,n}^\ell$  denote the collection of all  $\ell$ -bases in  $G$  and  $b^\ell(p, q, n)$  the total number of such sets. If  $\ell = 1$ , we simply write  $B_{p,q,n}$  and  $b(p, q, n)$ , and if  $p = 1$  or  $q = 1$  we use the notation  $G_{m,n}$ ,  $B_{m,n}^\ell$  and  $b^\ell(m, n)$  where  $m = p \cdot q$ . We consider also the 1-dimensional case in which we use notation  $B_n^\ell$  and  $b^\ell(n)$  since  $p = 1 = q$  and  $G = P_n$ , the  $n$ -vertex path.

In this paper we consider a few families of  $(p, q, n)$ -grid graphs such that  $p, q$  are fixed and  $p \leq q$  without loss of generality. We present recurrence formulas and generating functions describing the sequence  $(b^\ell(p, q, n))_{n \in \mathbb{N}}$  for the following cases:

1.  $p = 1, q = 1$  and any  $\ell \in \mathbb{N}$ ,
2.  $p = 1, q = 2$  and any  $\ell \in \mathbb{N}$ ,
3.  $p = 1, q = 3$  and  $\ell = 2$ ,
4.  $p = 2, q = 2$  and any  $\ell \in \mathbb{N}$ ,
5.  $p = 2, q = 3$  and  $\ell = 1$ .

Up to now there are only two publications [1, 2] on counting maximal independent sets (for  $\ell = 1$  only) on the path  $P_n$  and in the 2-dimensional grid graphs  $G_{m,n}$  with  $m \in \{2, 3, 4, 5\}$  [1]. As stated just above we present general results, that is for any natural  $\ell$ , on the numbers  $b^\ell(m, n)$  with  $m = 1, 2$  and  $b^\ell(p, q, n)$  with  $p = q = 2$ . Results in the latter case are stated in three theorems (for  $\ell = 1, 2$  or  $\ell \geq 3$ ). Proofs are nontrivial and rather complicated but made checkable due to our effort. So, it is very likely that any other general result can be overcomplicated. We will

apply the transfer matrix method as in [1] (see Stanley [5] for a basic reference), in particular in the cases 3, 4 and 5 listed above. All results presented in what follows have been checked by direct computer calculations. Additional results of the calculations, namely initial segments of sequences  $b(3, 3, n)$ ,  $b^2(3, 3, n)$  and  $b^3(3, 3, n)$ , are shown at the very end.

The following standard relation between a recurrence and the corresponding OGF (*ordinary generating function*) will be applied in what follows (without displaying details of calculations). The recurrence in question is linear homogeneous of order  $r$  with constant coefficients  $c_j$  with  $c_r \neq 0$  and  $c_0 = 1$ ,

$$a(n) + c_1 a(n - 1) + \dots + c_r a(n - r) = 0 \quad \text{for } n \geq r + 1.$$

The sequence  $a(n)$  is restricted to  $n \in \mathbb{N}$  and in fact  $a(n) := 0$  for  $n \leq 0$ . The corresponding rational function  $A(x) = P(x)/Q(x) = \sum_{n \geq 1} a'(n)x^n$  is the OGF of a sequence  $a'(n)$ . The two sequences coincide if coefficients of  $Q(x)$  agree with those in the recurrence,  $Q(x) = 1 + \sum_{j=1}^r c_j x^j$ , and  $P(x)$  is an appropriate polynomial, that is,  $P(x) = Q(x) \cdot A(x)$ . Consequently, the initial terms  $a(1), a(2), \dots, a(r)$  of the sequence determine the numerator of the OGF. Namely, if  $p_j$  are coefficients of  $P(x)$ ,  $P(x) = \sum_{j=0}^r p_j x^j$ , then  $p_0 = 0$  and  $p_m = a(m) + \sum_{j=1}^{m-1} c_j a(m - j)$  recursively for  $m = 1, 2, \dots, r$ .

By the way,  $x^r \cdot Q(1/x) = \sum_{j=0}^r c_j x^{r-j}$  is the characteristic polynomial of the recurrence.

## 2. $\ell$ -INDEPENDENCE ON PATHS

Recall that  $b^\ell(n)$  stands for the number of maximal  $\ell$ -independent vertex subsets of the path  $P_n$ .

**Theorem 2.1.** *Let  $a(n)$  be short for  $b^\ell(n)$ . Then*

$$(2.1) \quad a(n) = \sum_{i=1}^{\ell+1} a(n - \ell - i) \quad \text{for } n \geq 2\ell + 2,$$

with initial conditions

$$\begin{cases} a(j) = j & \text{for } j = 1, \dots, \ell, \ell + 1, \\ a(\ell + 1 + k) = \ell + 1 + k(k - 1)/2 & \text{for } k = 1, \dots, \ell. \end{cases}$$

The corresponding OGF follows.

$$B^\ell(x) = \frac{\sum_{j=1}^{\ell+1} jx^j + x^{\ell+1} \sum_{k=1}^{\ell} (\ell + 1 - k)x^k}{1 - \sum_{k=\ell+1}^{2\ell+1} x^k}.$$

**Proof.** Let  $a^*(n)$  count maximal  $\ell$ -independent sets on the path  $P_n$  such that the  $n$ th vertex is included in each set. Then clearly

$$(2.2) \quad a^*(j) = 1 \quad \text{for } j = 1, \dots, \ell, \ell + 1,$$

$$(2.3) \quad a^*(\ell + 1 + k) = k \quad \text{for } k = 1, \dots, \ell,$$

and the recurrence  $a^*(n) = \sum_{i=1}^{\ell+1} a^*(n - \ell - i)$  holds for  $n \geq 2\ell + 1$  provided that  $a^*(0) := 0$ . Consequently, on assuming  $a^*(k) := 0$  for  $k \leq 0$ , we extend validity of the recurrence to any  $n \geq \ell + 2$ ,

$$(2.4) \quad a^*(n) = \sum_{i=1}^{\ell+1} a^*(n - \ell - i) \quad \text{for } n \geq \ell + 2.$$

This agrees with (2.3) due to (2.2). Moreover, clearly

$$(2.5) \quad \begin{aligned} a(n) &= a^*(n) + a^*(n-1) + \dots + a^*(n-\ell) \quad (\text{for any } n > 0), \\ &= \sum_{i=1}^{\ell+1} a^*(n - \ell - i) + \sum_{i=1}^{\ell+1} a^*(n - 1 - \ell - i) + \dots \\ &+ \sum_{i=1}^{\ell+1} a^*(n - 2\ell - i) \end{aligned}$$

for  $n \geq 2\ell + 2$  due to (2.4), which on collecting  $i$ th term from each sum ( $i = 1, \dots, \ell + 1$ ) and due to (2.5) with  $n$  replaced by  $n - \ell - i$ , gives the terms on the right side of the recurrence (2.1) (for  $n \geq 2\ell + 2$ ). Initial values of  $a(j)$  with  $j > 0$  come via (2.5). Moreover,  $B^\ell(x) := \sum_{n \geq 1} a(n)x^n$  is the ordinary generating function (see OGF above) obtained from the recurrence. ■

**Remark 2.2.** Recurrence (2.1) with  $\ell = 1$  for  $n \geq 4$ , counting maximal independent sets on the  $n$ -vertex path  $P_n$ , is presented by Füredi [2] (without any proof). Essentially the same recurrence is independently presented in Euler [1, Sect. 3]. The corresponding sequence starting with  $a(1) = 1$  is A000931 (Padovan sequence) with offset 7 in [4].

**Remark 2.3.** The above proof is an example of a positioning method in recursive counting on paths [3].

### 3. CALCULATING $b^\ell(2, n)$

Given a  $(2, n)$ -grid graph  $G$  and  $\ell \in \mathbb{N}$  we will now present a recurrence formula for the calculation of  $b^\ell(2, n)$  for any  $n \in \mathbb{N}$ .

**Theorem 3.1.** For a given  $\ell \in \mathbb{N}$  and any  $n \geq 2\ell + 1$  we have the recurrence wherein  $a(k) := b^\ell(2, k)$ :

$$(3.1) \quad a(n) = a(n - \ell) + 2a(n - \ell - 1) + \dots + 2a(n - 2\ell + 1) + a(n - 2\ell),$$

with initial values

$$a(k) = 2k \text{ and } a(\ell + k) = 2\ell + 2k(k - 1),$$

for  $k = 1, \dots, \ell$ . The corresponding OGF follows.

$$\sum_{n \geq 1} b^\ell(2, n)x^n = \frac{\sum_{k=1}^\ell 2kx^k + \sum_{k=1}^{\ell-1} (2\ell - 2k)x^{\ell+k}}{1 - x^\ell - 2x^{(\ell+1)} - \dots - 2x^{(2\ell-1)} - x^{2\ell}}.$$

**Proof.** We first observe that, according to the structure of an  $\ell$ -basis within the last  $(\ell + 1)$  columns of  $G$ , for  $n \geq \ell + 2$  the collection  $B_{2,n}^\ell$  splits into  $a^i(n)$  many pairs of  $\ell$ -bases of type  $i$ ,  $i = 1, \dots, \ell + 1$ , as shown in Figure 1. Each pair comprises a basis and its upside-down image.



Figure 1. Bases representing each type.

Hence we have

$$(3.2) \quad a(n) = 2[a^1(n) + a^2(n) + \dots + a^\ell(n) + a^{\ell+1}(n)]$$

$$(3.3) \quad = a(n - 1) + a(n - 2) \quad \text{for } \ell = 1 \quad (\text{as in (3.1)})$$

since then  $2a^1(n) = a(n - 1)$  and  $2a^{\ell+1}(n) = a(n - 2)$  is easily seen, otherwise by inspection for  $\ell \geq 2$  and  $n \geq 2\ell + 2$ :

$$(3.4) \quad a^1(n) = a^\ell(n - 1),$$

$$(3.5) \quad a^i(n) = a^1(n - i + 1) + a^{\ell+1}(n - i + 1) \quad \text{for } i = 2, \dots, \ell,$$

$$a^{\ell+1}(n) = 2[a^{\ell+1}(n - \ell - 1) + a^1(n - \ell - 1) + \dots + a^{\ell-1}(n - \ell - 1)] + a^\ell(n - \ell - 1)$$

$$(3.6) \quad = a(n - \ell - 1) - a^\ell(n - \ell - 1) \quad (\text{by (3.2)}),$$

$$(3.7) \quad a^\ell(n - i) = a^i(n - \ell) \quad \text{for } i = 2, \dots, \ell - 1 \quad \text{if } \ell \geq 3.$$

Hence by (3.2), for  $\ell \geq 2$  we obtain

$$\begin{aligned} a(n) &= 2[(a^1(n - \ell) + a^{\ell+1}(n - \ell)) \quad (\text{by (3.3) and (3.5) for } i = \ell) \\ &\quad + (a^1(n - 1) + a^{\ell+1}(n - 1)) + \dots \quad (\text{by (3.5)}) \\ &\quad + (a^1(n - \ell + 1) + a^{\ell+1}(n - \ell + 1)) \\ &\quad + (a(n - \ell - 1) - a^\ell(n - \ell - 1))] \quad (\text{by (3.6)}). \end{aligned}$$

For  $\ell = 2$ , this has the form

$$\begin{aligned} a(n) &= 2[a^1(n-2) + a^3(n-2) + a^1(n-1)] \quad (= a(n-2) \text{ by (3.3) and (3.2)}) \\ &\quad + 2[a(n-4) - a^2(n-4)] \quad (\text{by (3.6)}) \\ &\quad + a(n-3) - a^2(n-3)] \\ &= a(n-2) + 2a(n-3) + a(n-4) \quad (\text{as in (3.1)}) \end{aligned}$$

because the remaining terms sum up to zero:  $a(n-4) - 2[a^2(n-3) + a^2(n-4)] = 0$  due to (3.2) and (3.5) with  $i = 2$  and with  $n - 3$  in place of  $n$ .

Otherwise  $\ell \geq 3$  and then using (3.3) or (3.6) we get

$$\begin{aligned} a(n) &= 2[a^1(n-\ell) + a^{\ell+1}(n-\ell) \\ &\quad + (a^\ell(n-2) + a(n-\ell-2) - a^\ell(n-\ell-2)) + \dots \\ &\quad + (a^\ell(n-\ell+1) + a(n-2\ell+1) - a^\ell(n-2\ell+1)) \\ &\quad + (a^\ell(n-\ell) + a(n-2\ell) - a^\ell(n-2\ell)) \\ &\quad + a(n-\ell-1) - a^\ell(n-\ell-1)]. \end{aligned}$$

We now use (3.2) in order to expand the difference  $a(n-2\ell) - 2a^\ell(n-2\ell)$ , also we use (3.7), and get

$$\begin{aligned} a(n) &= 2[a^1(n-\ell) + \dots + a^{\ell+1}(n-\ell)] \quad (= a(n-\ell) \text{ by (3.2)}) \\ &\quad + 2[a(n-\ell-1) + \dots + a(n-2\ell+1)] + a(n-2\ell) \\ &\quad + 2[(a^1(n-2\ell) + a^{\ell+1}(n-2\ell)) + a^2(n-2\ell) + \dots + a^{\ell-1}(n-2\ell)] \\ &\quad - 2[a^\ell(n-\ell-1) + a^\ell(n-\ell-2) + \dots + a^\ell(n-2\ell+1)] \end{aligned}$$

where  $\ell - 1$  pairs of summands, with both summands in the same position in the last two lines, cancel pair by pair, the first pair due to (3.5) with  $i = \ell$ , and all next due to (3.7) with  $n$  replaced by  $n - \ell$ . Thus the required recurrence

$$a(n) = a(n-\ell) + 2[a(n-\ell-1) + \dots + a(n-2\ell+1)] + a(n-2\ell)$$

for  $n > 2\ell$  is obtained. As to the initial values, we observe that for  $1 \leq n \leq \ell$  there are only 1-element  $\ell$ -bases in  $G$ , i.e.

$$a(n) = 2n \quad \text{for } n = 1, \dots, \ell,$$

and for  $n = (\ell + k)$  with  $k \leq \ell$  there are  $2(\ell - k)$   $\ell$ -bases of cardinality 1, and  $2(2i - 1)$  of cardinality 2 if we choose the first vertex in column  $(k - i + 1)$  with  $i \leq k$ . Altogether, this gives

$$a(\ell + k) = 2 \cdot \sum_{i=1}^k (2i - 1) + 2(\ell - k) = 2\ell + 2k(k - 1) \text{ for } k = 1, \dots, \ell.$$

Finally, the OGF can be found. ■

**Remark 3.2.** The case  $\ell = 1$  of Theorem 3.1 is proved in [1]. The corresponding sequence  $(b(2, n))_{n \geq 1}$  is the doubled Fibonacci sequence starting with  $b(2, 1) = 2$  at  $n = 1$ .

4. CALCULATING  $b^2(3, n)$

In this section we will show that already for  $\ell = 2$  and  $m = 3$ ,  $b^\ell(m, n)$  is difficult to calculate. To this end we adapt the transfer matrix method to our case by using the following rules.

**Rule 4.1.** Partition of all 2-bases in a  $(3, n)$ -grid, with  $n \geq 6$ , into 16 classes first, together with a multi-transformation of each class with  $n = k$  to classes with  $n = k + 1$  where  $k \geq 6$ .

**Rule 4.2.** Reducing the number of classes to 11. Therefore  $11 \times 11$  transfer matrix  $T$  is constructed such that each  $(i, j)$ -entry of  $T$  is a factor by which class  $j$  with  $k$  slices contributes to the cardinality of class  $i$  with  $k + 1$  slices in a grid,  $k \geq 6$ .

**Rule 4.3.** Cardinalities  $b^2(3, n)$  for  $n \leq 6$  are found by inspection. For  $n = 6$  cardinalities of classes are also found.

We obtain  $B_{3, k+1}^2$  from  $B_{3, k}^2$  by using the following result.

**Observation 4.1.** Recall that  $S_k$  stands for a slice of a grid. For each integer  $k \geq 2$  and any  $B \in B_{3, k+1}^2$  there exists  $B' \in B_{3, k}^2$  such that

$$(*) \quad \begin{cases} B' = B \text{ or else either } B' \text{ or } B' \setminus \{v'\} \text{ for some } v' \in B' \cap (S_{k-1} \cup S_k) \text{ is a} \\ \text{proper subset of } B \text{ and } B \setminus B' \subset S_{k+1}. \end{cases}$$

On the other hand, for each  $B' \in B_{3, k}^2$ , let  $\beta(B') = \{B \in B_{3, k+1}^2 \mid (*)\}$ . Thus a multi-transformation  $B' \mapsto B \in \beta(B')$  is obtained provided that  $B$  ranges over  $\beta(B')$ .

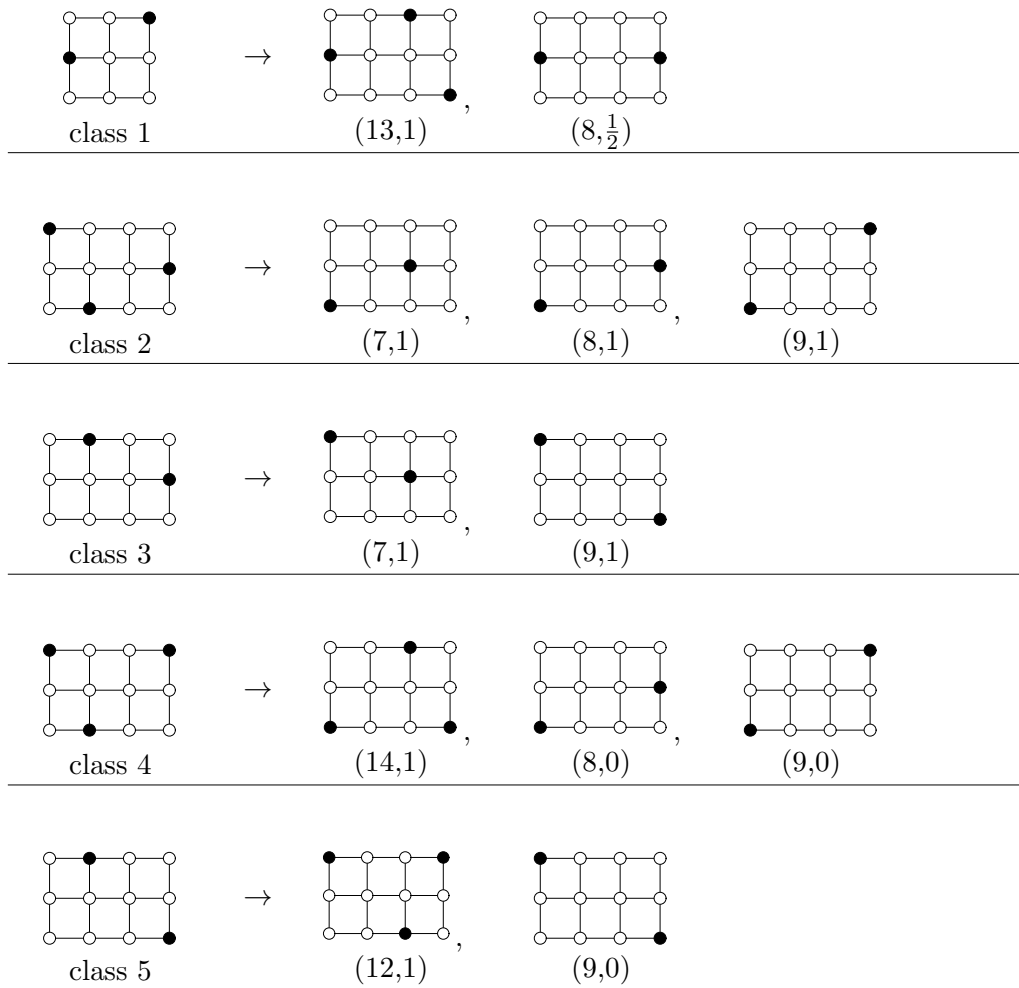
In other words, the symmetric difference of  $B$  and  $B'$  includes at most one element of either set. Additionally, if  $v'$  exists then it is in column  $k - 1$  or  $k$ . Moreover, if  $B \setminus B'$  is nonempty it comprises a vertex from column  $k + 1$ .

To make our approach as transparent as possible we partition  $B_{3, k}^2$  into 16 classes each of which is represented in figures below by a left-hand grid graph over 3, 4 or 5 columns together with an associated 2-independent set of black vertices. The interpretation is as follows: a 2-basis, say  $B'$ , in  $G_{3, n}$  with  $n \geq 6$  belongs to class  $i$  if vertices of  $B'$  in the last 3, 4 or 5 columns coincide (up to upside-down symmetry) with the black vertices in the figure for class  $i$ . At the same time the multi-transformation  $B' \mapsto B$  is presented. Namely, in the same figures, for each class  $i$  (at stage  $k$ ), an arrow indicates into which classes of the next stage

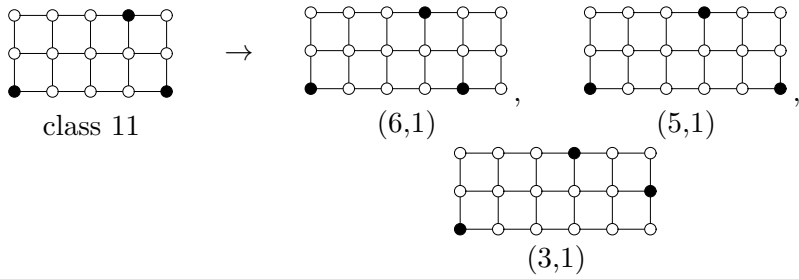
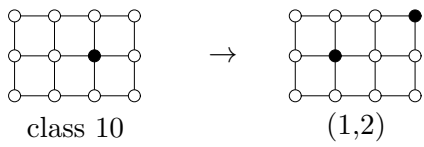
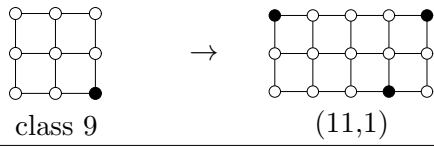
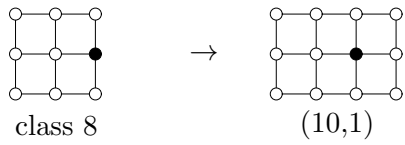
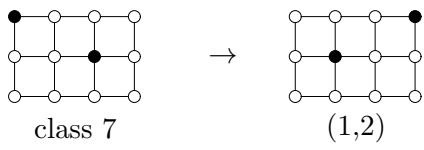
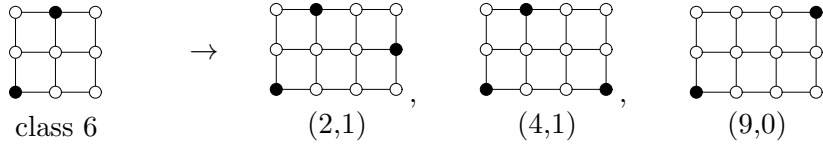
$k + 1$ , the class  $i$  is transformed by application of Observation 4.1, and by which factor,  $\frac{1}{2}$ , 1, 2, or 0 (0 if the contribution is already covered by another class, in general, a previous class), the cardinality changes. Just note that a factor of  $1/2$  applies when class 1 is transformed into class 8 since class 1 can be partitioned into pairs of bases which, due to upside-down symmetry, differ in column  $k$  only, and therefore both are transformed into the same basis of class 8, see  $t_{8,1} = 1/2$  in the matrix  $T$  below the following figures.

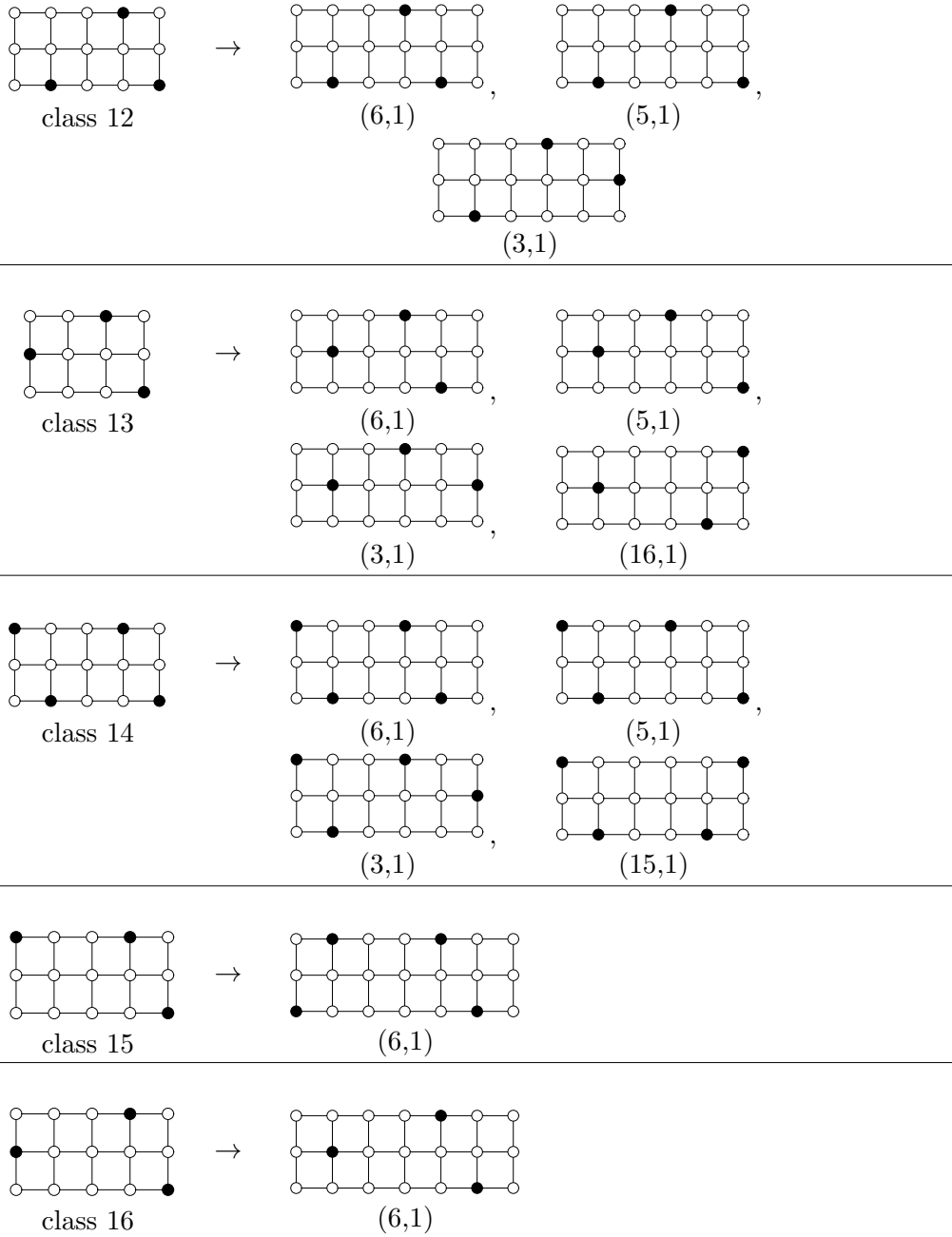
Note that only classes 1 and 6 are nonempty on  $n \geq 3$  columns. Classes 3 and 5 on 4 columns each are still empty. Classes 12 and 15 on 5 columns are empty. All classes are nonempty on  $n \geq 6$  columns. Class 8 on 5 columns and class 10 on 6 columns both have cardinality 3.

Definition of classes and multi-transformations:









Any two classes each of which contributes to the same classes with same factor are called *similar*. In what follows we merge similar classes into a new class. Thus we get new (primed) classes 7' (of 7 and 10), 9' (11 and 12) whence 5' (of 5 and 9), 10' (13 and 14) and 11' (15 and 16).

The transfer matrix  $T$  representing factors of contributions between (new) classes is presented in Table 1, see Rule 4.2 for the definition of  $T$ .

$T$ :

	1	2	3	4	5'	6	7'	8	9'	10'	11'
1							2				
2						1					
3									1	1	
4						1					
5'		1	1						1	1	
6									1	1	1
7'		1	1					1			
8	$\frac{1}{2}$	1									
9'					1						
10'	1			1							
11'										1	

Table 1. Transfer matrix  $T$  for  $b^2(3, n)$ .

Let  $C_n$  be a column vector of cardinalities of (new) classes in  $B^2(3, n)$  for  $n \geq 6$ . The vector  $C_6$  is found by inspection. For  $n > 6$ , the vectors are obtained from the formula  $C_{6+k} = T^k \cdot C_6$  where  $k \in \mathbb{N}$  (see Table 2).

Values of  $b^2(3, n)$  for  $n < 6$  are obtained by inspection, see Table 3.

However, for  $n \geq 6$ ,  $b^2(3, n)$  is equal to the sum of components in  $C_n$ , see Tables 2 and 3 for ten initial values. The following determinant  $\det(I - xT) = 1 - x^2 - 3x^3 - 4x^4 - x^5 - x^6 + x^7 + 2x^8 + x^9 + x^{10}$ , which is a polynomial of degree 10, and ten initial values lead to the first generating function

$$g(x) = \frac{3x + 4x^2 + 8x^3 + 4x^4 + x^5 - 5x^7 - 3x^8 - 3x^9 - x^{10}}{1 - x^2 - 3x^3 - 4x^4 - x^5 - x^6 + x^7 + 2x^8 + x^9 + x^{10}}.$$

This function can be simplified by a factor  $(x + 1)$  so that we obtain the following result.

**Theorem 4.2.** *Let  $b^2(3, n)$  be the number of maximal 2-independent sets in the planar  $3 \times n$  grid graph. Then*

$$\sum_{n \geq 1} b^2(3, n)x^n = \frac{3x + x^2 + 7x^3 - 3x^4 + 4x^5 - 4x^6 - x^7 - 2x^8 - x^9}{1 - x - 3x^3 - x^4 - x^6 + 2x^7 + x^9},$$

providing the recurrence for  $a(n) = b^2(3, n)$ ,  $a(n) = a(n - 1) + 3a(n - 3) + a(n - 4) + a(n - 6) - 2a(n - 7) - a(n - 9)$  for  $n \geq 10$ , with initial values as in Table 3.

Classes	$n$				
	6	7	8	9	10
1	6	18	28	54	110
2	4	8	16	28	58
3	6	12	22	48	86
4	4	8	16	28	58
5'	12	22	42	86	162
6	8	16	28	58	112
7'	9	14	27	55	106
8	4	7	17	30	55
9'	6	12	22	42	86
10'	6	10	26	44	82
11'	4	6	10	26	44
$\Sigma$	69	133	254	499	959

Table 2. Column vectors  $C_n$ .

$n$	1	2	3	4	5	6	7	8	9
$b^2(3, n)$	3	4	11	17	36	69	133	254	499

Table 3. Beginning values of  $b^2(3, n)$ .

### 5. CALCULATING $b^\ell(2, 2, n)$

Grid graphs are usually studied in 2 dimensions since the main field of applications is statistical physics. Counting techniques, however, still work for 3 dimensions as we are now going to show for the first example:  $(2, 2, n)$ -grids. For any considered case ( $\ell = 1, 2$  and  $\ell \geq 3$ ) we use the transfer matrix method as outlined in section 4. Moreover, the multi-transformation  $B' \mapsto B \in \beta(B')$  (Observation 4.1) from an  $\ell$ -basis  $B'$  with  $n = k$  to  $\ell$ -basis  $B$  with  $n = k + 1$  may involve adjustment within a part of  $B'$  comprising last  $\ell$  slices  $S_j, j = k, k - 1, \dots, k - \ell + 1$ . In the following sections, classes of bases are defined up to isometry of the 3-dimensional grid, respecting the numbering of slices.

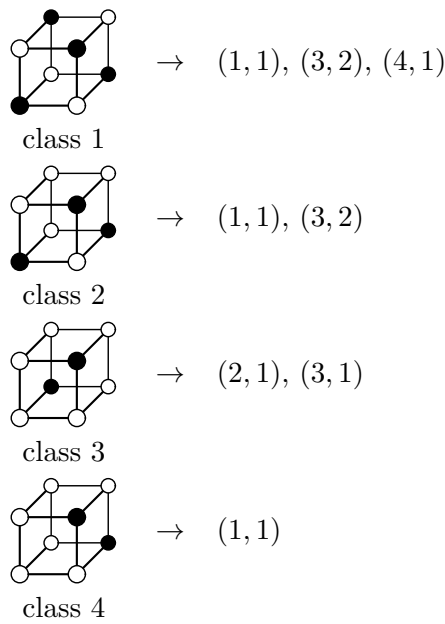
#### 5.1. Case $\ell = 1$

We partition  $B_{2,2,k}$  into 4 classes for  $k \geq 3$  according to the structure of the bases within the last 2 slices. The following figures present definitions of classes, each arrow indicates a multi-transformation, and in each integer pair  $(a, b)$ ,  $a$  is the number of a class and  $b$  is a contribution factor. Those factors are the only

nonzero items in the following transfer matrix  $T$ , where  $t_{a,j} = b$  if class  $j \rightarrow (a, b)$ , see Rule 4.2.

$$T = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 2 & 2 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Definition of classes and multi-transformations:



Since  $\det(I - xT) = 1 - 2x - 2x^2 + x^3 + 2x^4$  is of degree 4, we need four initial values of the sequence  $(b^1(2, 2, n))_{n \in \mathbb{N}}$  in order to find its generating function. Note that the 4-cycle is a slice in our case and therefore  $b^1(2, 2, 1) = 2$  is easily seen. As in section 4,  $C_n$  is a column vector of cardinalities of classes in  $B^1(2, 2, n)$  for  $n \geq 2$ . The vector  $C_2$ , found by inspection, is presented in Table 4. For  $n > 2$ ,  $C_n$  is obtainable from the formula  $C_{2+k} = T^k C_2$ . Summing up components of  $C_n$  we get  $b^1(2, 2, n)$ , see Table 4 for  $n = 3, 4$ . Hence we get the generating function

$$g(x) = \frac{2x + 2x^2 - 4x^4}{1 - 2x - 2x^2 + x^3 + 2x^4},$$

which simplifies by a factor  $1 - x$ . Consequently, the following result is obtained.

**Theorem 5.1.1.** *Let  $b^1(2, 2, n)$  be the count of maximal independent sets in the 3-dimensional  $(2, 2, n)$  grid graph. Then*

$$\sum_{n \geq 1} b^1(2, 2, n)x^n = \frac{2x + 4x^2 + 4x^3}{1 - x - 3x^2 - 2x^3}.$$

In the resulting recurrence

$$a(n) = a(n - 1) + 3a(n - 2) + 2a(n - 3) \text{ for } n \geq 4,$$

$a(n) = b^1(2, 2, n)$  if the initial values of  $a(n)$  are as follows:

$$a(1) = b^1(2, 2, 1) = 2, \quad a(2) = b^1(2, 2, 2) = 6, \quad a(3) = b^1(2, 2, 3) = 16.$$

classes	n		
	2	3	4
1	2	2	8
2	0	4	8
3	4	8	20
4	0	2	2
$\Sigma$	6	16	38

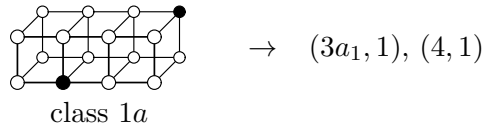
Table 4. Column vectors  $C_n$ .

n	1	2	3	4	5	6	7	8	9	10
$b^1(2, 2, n)$	2	6	16	38	98	244	614	1542	3872	9726

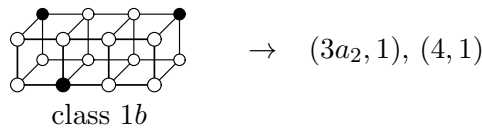
Table 5. Beginning values of  $b^1(2, 2, n)$ .

**5.2. Case  $\ell = 2$**

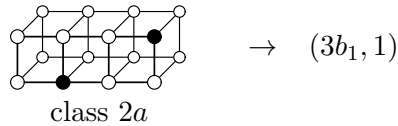
Definition of classes and multi-transformations:



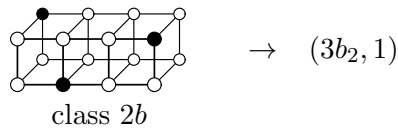
$$\rightarrow (3a_1, 1), (4, 1)$$



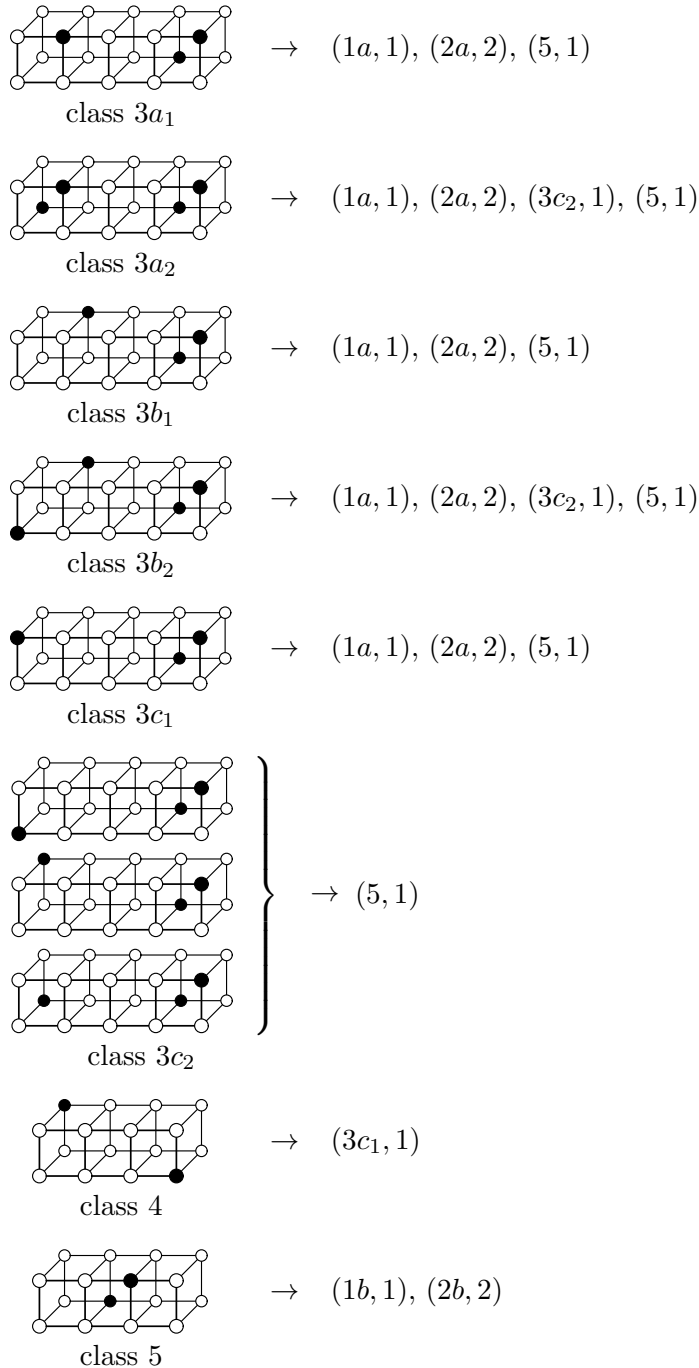
$$\rightarrow (3a_2, 1), (4, 1)$$



$$\rightarrow (3b_1, 1)$$



$$\rightarrow (3b_2, 1)$$



Merging similar classes and renaming gives the following new classes:  $3a$  (from  $3a_1, 3b_1, 3c_1$ ),  $3b$  ( $3a_2, 3b_2$ ) and  $3c$  ( $3c_2$ ). Hence the transfer matrix  $T$  (of size  $9 \times 9$ ) is obtained. Initial values of  $b^2(2, 2, n)$  for  $n = 1, \dots, 4$  as well as an initial

vector  $C_5$  of the class cardinalities are obtained by inspection, see Tables 7 and 8.

$T:$

	$1a$	$1b$	$2a$	$2b$	$3a$	$3b$	$3c$	4	5
$1a$					1	1			
$1b$									1
$2a$					2	2			
$2b$									2
$3a$	1		1					1	
$3b$		1		1					
$3c$						1			
4	1	1							
5					1	1	1		

Table 6. Transfer matrix  $T$  for  $b^2(2, 2, n)$ .

Classes	$n$		
	5	6	7
$1a$	12	16	52
$1b$	4	12	16
$2a$	24	32	104
$2b$	8	24	32
$3a$	4	40	64
$3b$	12	12	36
$3c$	0	12	12
4	4	16	28
5	12	16	64
$\Sigma$	80	180	408

Table 7. Column vectors  $C_n$ .

Calculation gives  $\det(I - xT) = 1 - 3x^2 - 4x^3 - 4x^4 + 9x^6 + 3x^7$ . This polynomial implies the required recurrence (of order 7) and is the denominator of the required OGF. Hence, using initial values as in Table 8 leads to the following.

**Theorem 5.2.1.** *Let  $b^2(2, 2, n)$  count the maximal 2-independent sets in the  $(2, 2, n)$  grid. Then*

$$\sum_{n \geq 1} b^2(2, 2, n)x^n = \frac{4x + 4x^2 + 8x^3 + 4x^4 - 12x^5 - 12x^6 - 4x^7}{1 - 3x^2 - 4x^3 - 4x^4 + 9x^6 + 3x^7}$$





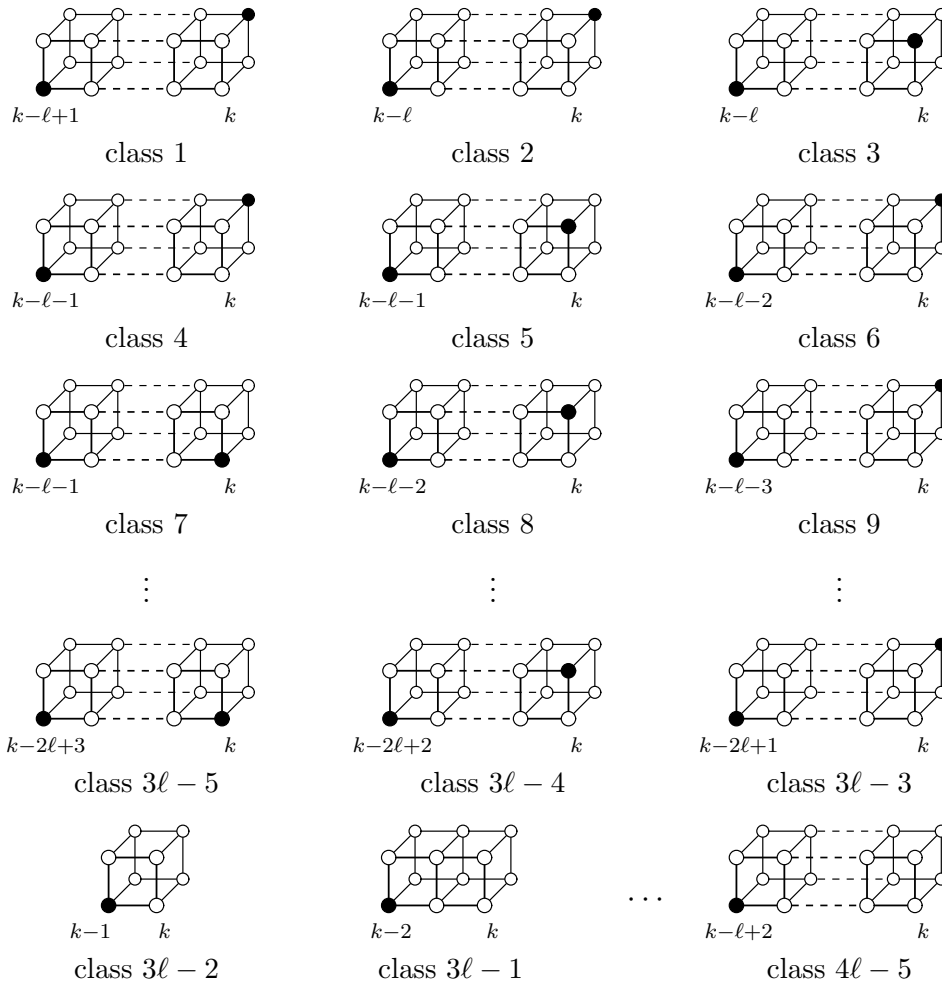
- Class 1  $\rightarrow (2,1), (3,2), (10,1)$
- Class 2  $\rightarrow (4,1), (7,1), (10,1)$
- { Class 3  $\rightarrow (5,1), (10,1)$
- { Class 4  $\rightarrow (6,1), (10,1)$
- { Class 5  $\rightarrow (8,1), (10,1)$
- { Class 6  $\rightarrow (9,1), (10,1)$
- { Class 7  $\rightarrow (10,1)$
- { Class 8  $\rightarrow (10,1)$
- { Class 9  $\rightarrow (10,1)$
- Class 10  $\rightarrow (11,1)$
- Class 11  $\rightarrow (1,1)$

	1	2	3'	4'	5'	6'	7'
1							1
2	1						
3'	2	1					
4'			1				
5'		1		1			
6'	1	1	1	1	1		
7'						1	

(a) Multi-transformations

(b) Transfer matrix  $T$

Table 10. Case  $\ell = 4$ .



The resulting transfer matrix is of size  $(2\ell - 1) \times (2\ell - 1)$  and is presented in Table 11.

$$T = \left[ \begin{array}{cccccc|cccc} 0 & \dots & & & & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & & & 0 & 0 & \dots & & 0 \\ 2 & 1 & 0 & \dots & & 0 & 0 & \dots & & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 & \vdots & & & \vdots \\ 0 & 1 & 0 & 1 & 0 & \dots & 0 & & & \\ 0 & 0 & 0 & 0 & 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & & & & \ddots & \ddots & \ddots & \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & & 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & \dots & & 1 & 1 & 1 & 0 & 0 & \dots & 0 \\ \hline 0 & \dots & & & & 0 & 1 & 0 & \dots & & 0 \\ 0 & \dots & & & & 0 & 0 & 1 & 0 & \dots & 0 \\ \vdots & & & & & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & & & & 0 & 0 & \dots & 0 & 1 & 0 \end{array} \right] \left. \vphantom{\begin{array}{c} \vdots \\ \vdots \\ \vdots \end{array}} \right\} \ell - 3$$

Table 11. Transfer matrix of size  $(2\ell - 1) \times (2\ell - 1)$  for  $\ell \geq 3$ .

We are going to prove the following formula (and its generalization):

$$(5.3.1) \quad (\ell = 3) \quad \det(I - xT) = 1 - x^2 - 3x^3 - 3x^4 - x^5.$$

Note that the following recurrence is implied for  $\ell = 3$ :

$$(5.3.2) \quad a(n) = a(n - 2) + 3a(n - 3) + 3a(n - 4) + a(n - 5).$$

In order to evaluate  $\det(I - xT)$  we consider submatrices  $B_1, \dots, B_{\ell-1}$  of size from  $(2\ell - 4) \times (2\ell - 4)$  to  $(\ell - 2) \times (\ell - 2)$ , respectively. All of them reside in the lower right corner of the matrix obtained from  $I - xT$  by deleting the last column, see Table 12.

We first show the following result.

**Lemma 5.3.1.** *For any  $\ell \geq 3$ ,*

$$(5.3.3) \quad \det(I - xT) = 1 - (x^3 + 2x^2) \det(B_1) + x^2 \det(B_2) - x^{\ell-1}.$$

$$I - xT = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & -x \\ -x & 1 & 0 & 0 & 0 & 0 & 0 \\ -2x & -x & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \underbrace{\begin{bmatrix} -x & 1 & 0 & 0 \\ 0 & -x & 1 & 0 \\ -x & -x & -x & 1 \\ 0 & 0 & 0 & -x \end{bmatrix}}_{B_1} & 0 & 0 & 0 \\ 0 & -x & 0 & -x & 1 & 0 & 0 \\ -x & -x & -x & -x & -x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -x & 1 \end{bmatrix} \ell - 3 (= 1)$$

Table 12. The matrix  $I - xT$  for  $\ell = 4$  (and submatrices  $B_1, B_2, B_3$ ).

**Proof.** Throughout the proof each variant of “expanding a determinant” means that the determinant is to be expanded according to the elements of the first row. Note that expanding our determinant gives  $\det(I - xT) = 1 - xM$  where  $M$  stands for a respective minor,  $M = M_{1,2\ell-1}$ . We now move the factor  $-x$  to the first column of  $M$  and expand the resulting determinant. We now continue moving each numerical factor at a minor to the first column, we next sum up the two available determinants (since they differ in the first column only), and what results is expanded. This gives an auxiliary equality

$$-xM = -(x^3 + 2x^2) \det(B_1) - D$$

where  $D$  is a determinant of order  $2\ell - 4$ . On expanding  $D$  we (split the first column of the resulting determinant and) split the determinant itself into two summands, and get  $-D = x^2 \det(B_2) + (-1)^{1+\ell-2}(-x^2)(-x)^{\ell-3}$ , which ends the proof of (5.3.3). ■

**Remark 5.1.** The case  $\ell = 3$  is included in the general formula due to the following trivial calculation:

$$-D = \det([-x^3 - x^2]) = x^2 \det([-x]) - x^2,$$

since then  $B_2 = [-x]$ .

It is easily seen, cf. Table 12, that

$$\det(B_{\ell-1}) = (-x)^{\ell-2}$$

and for  $j = 1, \dots, \ell - 2$ ,

$$\det(B_j) = -x \det(B_{j+1}) + (-1)^{\ell-1-j}(-x)^{\ell-2}.$$

Therefore after substituting we obtain

$$\begin{aligned}
 \det(B_{\ell-2}) &= (-x)^{\ell-1} + (-1)(-x)^{\ell-2} \\
 \det(B_{\ell-3}) &= (-x)^\ell + (-1)(-x)^{\ell-1} + (-1)^2(-x)^{\ell-2} \\
 \det(B_{\ell-4}) &= (-x)^{\ell+1} + (-1)(-x)^\ell + (-1)^2(-x)^{\ell-1} + (-1)^3(-x)^{\ell-2} \\
 &\vdots \\
 \det(B_2) &= (-x)^{2\ell-5} + (-1)(-x)^{2\ell-6} + (-1)^2(-x)^{2\ell-7} + \dots \\
 &\quad + (-1)^{\ell-3}(-x)^{\ell-2} \\
 \det(B_1) &= (-x)^{2\ell-4} + (-1)(-x)^{2\ell-5} + (-1)^2(-x)^{2\ell-6} + \dots \\
 &\quad + (-1)^{\ell-2}(-x)^{\ell-2}
 \end{aligned}$$

and equation (5.3.3) becomes

$$\begin{aligned}
 \det(I - xT) &= 1 + (-x)^{2\ell-1} + (-1)(-x)^{2\ell-2} + (-1)^2(-x)^{2\ell-3} + \dots \\
 &\quad + (-1)^{\ell-2}(-x)^{\ell+1} + (-2)(-x)^{2\ell-2} + (-2)(-1)(-x)^{2\ell-3} \\
 &\quad + (-2)(-1)^2(-x)^{2\ell-4} + \dots + (-2)(-1)^{\ell-2}(-x)^\ell + (-x)^{2\ell-3} \\
 &\quad + (-1)(-x)^{2\ell-4} + (-1)^2(-x)^{2\ell-5} + \dots + (-1)^{\ell-3}(-x)^\ell \\
 &\quad + (-1)^\ell(-x)^{\ell-1} \\
 &= 1 - x^{\ell-1} - 3x^\ell - 4x^{\ell+1} - \dots - 4x^{2\ell-5} - 4x^{2\ell-4} - 4x^{2\ell-3} \\
 &\quad - 3x^{2\ell-2} - x^{2\ell-1} \quad (\text{irreducible for } \ell = 3, 4, 5),
 \end{aligned}$$

providing the recurrence

$$\begin{aligned}
 (5.3.4) \quad a(n) &= a(n - \ell + 1) + 3a(n - \ell) + 4a(n - \ell - 1) + \dots \\
 &\quad + 4a(n - 2\ell + 3) + 3a(n - 2\ell + 2) + a(n - 2\ell + 1)
 \end{aligned}$$

for  $n \geq 2\ell$  and  $\ell \geq 3$ .

Note that formula (5.3.4), when carefully reduced, really gives (5.3.2) found for  $\ell = 3$ .

We still have to determine the initial values in order to have  $a(n) = b^\ell(2, 2, n)$  for  $\ell \geq 3$ . To this end, we observe that for  $n = \ell + k$  with  $1 \leq k \leq \ell - 1$ , the family  $B_{2,2,\ell+k}^\ell$  contains four types of bases, depicted in Figure 2. For  $n = 1, \dots, \ell - 1$  all bases are of type 4, and we obtain  $a(n) = 4n$ . For  $n = \ell$ , there are four bases of type 1 and  $4(\ell - 2)$  bases of type 4 leading to  $a(n) = 4(n - 1)$ . To determine  $a(n)$  for  $n = \ell + k$ , we first let  $k$  run from 1 to  $\ell - 2$ . We find a total number of  $4[(k + 1) + k + \dots + 1] + 8[k + (k - 1) + \dots + 1] + 4[(k - 1) + (k - 2) + \dots + 1] + 4[(\ell + k)((\ell + k) - (\ell - 1))]$  bases of the four types, yielding  $a(\ell + k) = 4(\ell + 2k^2 + k - 1)$  for  $k = 1, 2, \dots, \ell - 2$ .

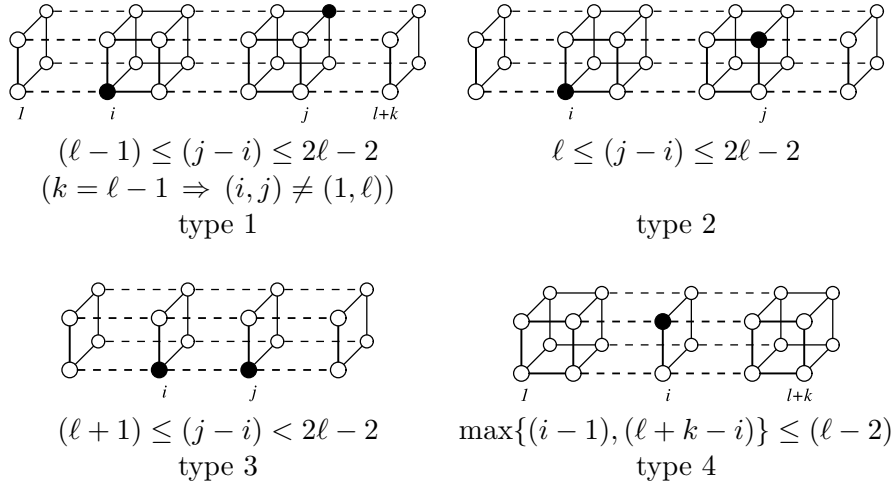


Figure 2. Types of bases of  $B_{2,2,\ell+k}^{\ell}$ ,  $1 \leq k \leq \ell - 1$ .

Finally, if  $k = \ell - 1$ ,  $B_{2,2,2\ell-1}^{\ell}$  does not contain a basis of type 1 for  $(i, j) = (1, \ell)$  nor a basis of type 3 for  $(j - i) = 2\ell - 2$ , and there is no basis of type 4. Subtracting 4 from the above value for  $k = \ell - 1$ , gives

$$a(2\ell - 1) = 4(2\ell^2 - 2\ell - 1).$$

By evaluating  $(1 - x^{\ell-1} - 3x^{\ell} - 4x^{\ell+1} - \dots - 4x^{2\ell-3} - 3x^{2\ell-2} - x^{2\ell-1})g(x)$  we obtain the associated generating function  $g(x)$  as a rational function.

Our results on  $(2, 2, n)$ -grids can be summarized as follows.

**Theorem 5.3.1.** *Given  $\ell \geq 3$  and any  $n \geq 2\ell$ , on defining  $a(n) = b^{\ell}(2, 2, n)$ , we have the recurrence*

$$\begin{aligned}
 a(n) &= a(n - \ell + 1) + 3a(n - \ell) + 4a(n - \ell - 1) + \dots \\
 &\quad + 4a(n - 2\ell + 3) + 3a(n - 2\ell + 2) + a(n - 2\ell + 1),
 \end{aligned}$$

with initial values

- $a(k) = 4k$  for  $k = 1, \dots, \ell - 1$ ,
- $a(\ell + k) = 4(\ell + 2k^2 + k - 1)$  for  $k = 0, \dots, \ell - 2$ ,
- $a(2\ell - 1) = 4(2\ell^2 - 2\ell - 1)$ ,

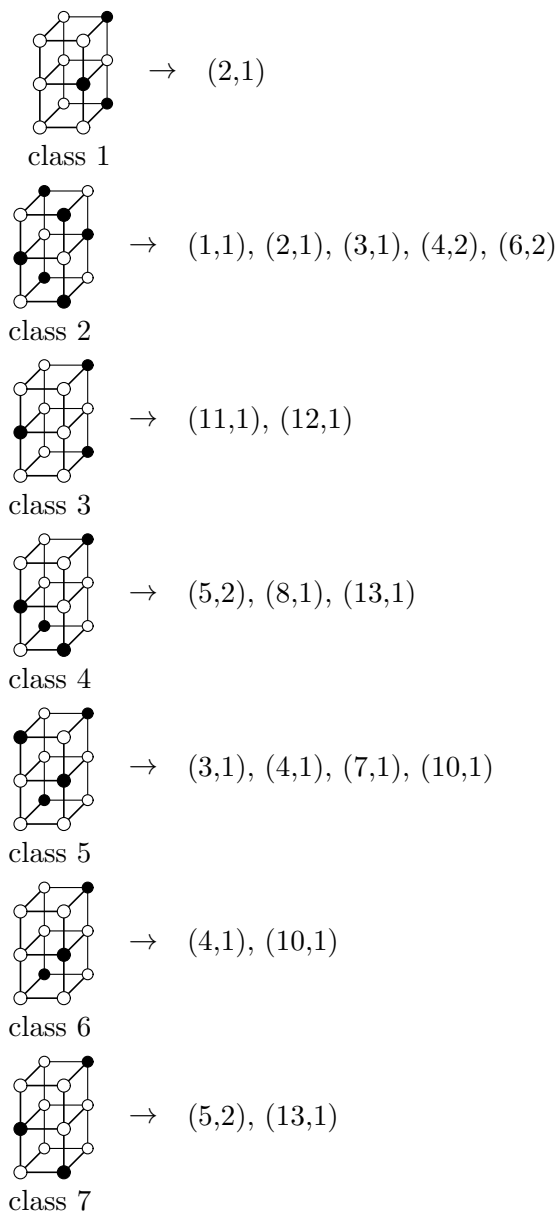
and the generating function

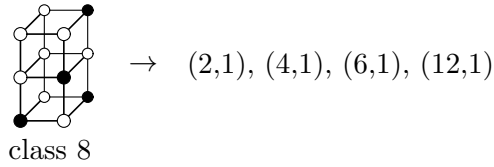
$$\sum_{n \geq 1} a(n)x^n = \frac{\sum_{k=1}^{\ell-1} 4kx^k + \sum_{k=0}^{\ell-3} 4(\ell - k - 2)x^{\ell+k}}{1 - x^{\ell-1} - 3x^{\ell} - 4x^{\ell+1} - \dots - 4x^{2\ell-3} - 3x^{2\ell-2} - x^{2\ell-1}}.$$

6. THE CASE  $p = 2, q = 3, \ell = 1$

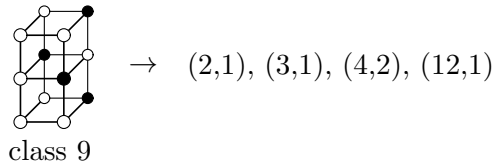
In this case we partition  $B_{2,3,k}$  into classes according to the structure of the bases within the last 2 slices. Note that any slice  $S_k$  of  $G_{2,3,k}$  contains altogether 17 distinct independent sets. We get 13 classes up to isometry.

Definition of classes and multi-transformations:

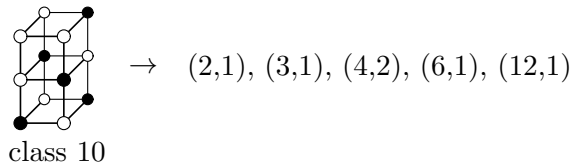




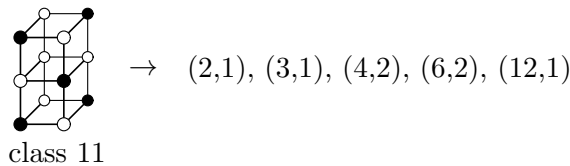
$$\rightarrow (2,1), (4,1), (6,1), (12,1)$$



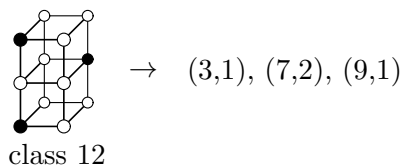
$$\rightarrow (2,1), (3,1), (4,2), (12,1)$$



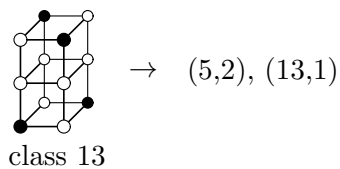
$$\rightarrow (2,1), (3,1), (4,2), (6,1), (12,1)$$



$$\rightarrow (2,1), (3,1), (4,2), (6,2), (12,1)$$



$$\rightarrow (3,1), (7,2), (9,1)$$



$$\rightarrow (5,2), (13,1)$$

On merging classes 7 and 13 into a new class 7' we get a transfer matrix  $T$ , see Table 13.

Calculating determinant of  $I - xT$  gives us

$$(6.1) \quad \det(I - xT) = (1 - 2x - 9x^2 + 2x^3 + 17x^4 + 4x^5 - 8x^6 + 3x^7 - x^8 + 3x^9 + 2x^{10} - 4x^{11}).$$

Initial values of  $(b(2, 3, n))_{n \geq 1}$  are obtained from direct calculation and from initial cardinalities of the classes, which are presented in Table 14. So, we get

$$(6.2) \quad (b(2, 3, n))_{n \geq 1} = (4, 16, 66, 244, 968, 3726, 14520, 56352, 218978, 850620, 3304624, \dots)$$

Thus we have arrived at the following result.



$T:$

	1	2	3	4	5	6	7'	8	9	10	11	12
1		1										
2	1	1						1	1	1	1	
3		1			1				1	1	1	1
4		2			1	1		1	2	2	2	
5				2			2					
6		2						1		1	2	
7'				1	1		1					2
8				1								
9												1
10					1	1						
11			1									
12		1	1					1	1	1	1	

Table 13. Transfer matrix for  $b(2, 3, n)$ .

**Theorem 6.1.** *Let  $b(2, 3, n)$  count the maximal independent sets in the  $(2, 3, n)$  grid. Then*

$$\sum_{n \geq 1} b(2, 3, n)x^n = \frac{4x + 8x^2 - 2x^3 - 24x^4 - 14x^5 + 14x^6 - 2x^7 + 10x^8 - 6x^9 - 8x^{10}}{1 - 2x - 9x^2 + 2x^3 + 17x^4 + 4x^5 - 8x^6 + 3x^7 - x^8 + 3x^9 + 2x^{10} - 4x^{11}}$$

is the OGF, providing the recurrence for  $a(n) = b(2, 3, n)$

$$(6.3) \quad \begin{aligned} a(n) &= 2a(n - 1) + 9a(n - 2) - 2a(n - 3) - 17a(n - 4) \\ &\quad - 4a(n - 5) + 8a(n - 6) - 3a(n - 7) + a(n - 8) \\ &\quad - 3a(n - 9) - 2a(n - 10) + 4a(n - 11) \end{aligned}$$

for  $n > 11$ , with initial values  $a(1), \dots, a(11)$  given in (6.2).

## 7. COMPUTER AIDED VERIFICATION AND FUTURE WORK

In this paper we have shown how to adapt the transfer matrix method to count maximal  $\ell$ -independent sets in several classes of grid graphs. A sophisticated partition of these sets into classes for a fixed size of the graph and a detailed analysis of the resulting transfer matrix have been at the basis of our approach. In addition, we have tried to push the values  $p$ ,  $q$  and  $\ell$  as high as possible. Finally, all results presented in the previous sections have been checked by computer calculations. To get maximal certainty two different algorithms have been implemented.

classes	$n$								
	3	4	5	6	7	8	9	10	11
1	2	2	16	54	218	852	3298	12850	49880
2	2	16	54	218	852	3298	12850	49880	193838
3	8	26	110	404	1606	6174	24080	93394	363046
4	8	40	156	600	2352	9100	35416	137504	534292
5	12	44	164	652	2492	9748	37740	146812	569988
6	4	16	72	260	1048	4024	15700	60920	236776
7'	14	42	170	646	2522	9770	37990	147490	573130
8	4	8	40	156	600	2352	9100	35416	137504
9	2	4	22	78	312	1202	4686	18172	70662
10	4	16	60	236	912	3540	13772	53440	207732
11	2	8	26	110	404	1606	6174	24080	93394
12	4	22	78	312	1202	4686	18172	70662	274382
$\Sigma$	66	244	968	3726	14520	56352	218978	850620	3304624

Table 14. Class cardinalities for  $b(2, 3, n)$ .

The first is based on classical technique of searching a domain for possible values and filtering out elements fulfilling a number of prescribed criteria. This kind of algorithms are generally of exponential time complexity since the search space is a set of subsets. In our case it turned out to be very time-consuming, in spite of the use of sophisticated reduction techniques, and therefore only small size instances could be handled efficiently. The second algorithm uses transfer matrices that are generated completely automatically but in a different manner than described above and in [1]. The upcoming matrices were of huge size but we still could use them to compute the numbers  $b^\ell(p, q, n)$  in a direct way. Our second algorithm has also been used to calculate additional results. Some of them, for cases  $b(3, 3, n)$ ,  $b^2(3, 3, n)$ ,  $b^3(3, 3, n)$  and  $n = 1, \dots, 12$ , are presented in Table 15. It is an open problem to fully describe the sequences  $(b^\ell(3, 3, n))_{n \geq 1}$  for any  $\ell > 0$ .

The results presented in this paper can be generalized. Since any grid graph can be defined as a *Cartesian product* of graphs, a large family of graphs interesting for generalization is at hand. Another subject for future work could be the study of the asymptotic behaviour of the number  $a(n)$  in terms of  $n$  and distance parameter  $\ell$  when  $a(n)$  is completely determined as in Theorems 2.1, 3.1 or 5.3.1. In the case when  $\ell$  is fixed, we have omitted asymptotic estimates of the form  $a(n) = \Theta(\lambda^n)$  where  $\lambda$  is the dominant characteristic root of the corresponding recurrence and its reciprocal  $1/\lambda$  is the dominant pole of the OGF,  $\lambda > 1$ .

$n$	$\ell = 1$	$\ell = 2$	$\ell = 3$
1	10	11	7
2	66	46	26
3	496	182	57
4	3556	1026	190
5	26948	4836	646
6	199898	23922	1914
7	1491120	118674	5960
8	11087686	584516	18824
9	82651544	2889306	58248
10	615619076	14266546	181196
11	4584511168	70455052	565328
12	34147089394	347980122	1759720

Table 15. Values of  $b^\ell(3, 3, n)$  obtained with computer.

### Acknowledgements

We are grateful to the referees for many valuable suggestions.

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doi:10.1017/CBO9780511805967

Received 31 January 2012  
 Revised 11 October 2012  
 Accepted 5 November 2012

