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# COUNTING PERFECT MATCHINGS IN POLYOMINOES WITH AN APPLICATION TO THE DIMER PROBLEM

*Abstract.* A *polyomino* is a connected finite plane graph with no cut-points in which all interior regions (called *cells*) are unit squares. Let $P$ be a given polyomino and $e$ be a given edge of $P$. A simple algorithm is developed for calculating the numbers $m(P)$ and $m(P, e)$ of all perfect matchings of $P$ and of those perfect matchings of $P$ which contain the edge $e$, respectively.

The numbers $m(P)$ and $m(P, e)/m(P)$ play an important role in the dimer problem of statistical crystal physics.

**1. Introduction.** The dimer problem has its origin in the investigation of the thermodynamic properties of a system of diatomic molecules (called *dimers*) adsorbed on the surface of a crystal (see, e.g., [1] and [9]–[11]). In many cases, the most favourable points for the adsorption of atoms form a part $L$ of a square lattice and a dimer can occupy two neighbouring points of $L$ (and only such points). A *dimer covering* is an arrangement $C$ of dimers on $L$ such that every dimer of $C$ occupies two neighbouring points and every point of $L$ is covered by exactly one dimer of $C$. Let us identify the point set of $L$ with the vertex set of a graph $P$ corresponding to $L$ (Fig. 1a); $P$ is a special polyomino (for the definition see the Abstract; more about polyominoes in [4]). To any dimer covering of $L$ there corresponds a *perfect matching* (PM) $M$ of $P$ (i.e., a set of disjoint edges covering all vertices of $P$), and conversely (Fig. 1b).

Let $x$, $y$ be two neighbouring points in $L$ and let $e = (x, y)$ be the edge connecting $x$ and $y$ in $P$. Suppose that every dimer covering of $L$ occurs with the same probability. The physicist is interested in the number $m_L$ of all dimer coverings of $L$ and in the probability $p_L(x, y)$ to find $x$ and $y$ covered by the same dimer in a randomly chosen covering. Let $m(G)$ and $m(G, e)$ denote the numbers of all PMs of a graph $G$ and of those PMs of $G$ which contain the edge $e$, respectively. Clearly,

$$m_L = m(P) \quad \text{and} \quad p_L(x, y) = m(P, e)/m(P);$$

further,

$$m(P, e) = m(P-\{x, y\}) = m(P)-m(P-e),$$

where $P-e$ and $P-\{x, y\}$ denote the subgraphs of $P$ obtained from $P$ by omitting the edge $e$ or the vertices $x$ and $y$ and all edges incident to them, respectively. However, in general, $P-e$ and $P-\{x, y\}$ are no longer polyominoes; therefore, we shall extend our investigations to a certain class $S$ of subgraphs of polyominoes (see Section 3). The problem of determining $m_L$ and $p_L(x, y)$ will be considered to be solved as soon as we have a handy method (an algorithm) for calculating $m(G)$ for every graph $G \in S$.

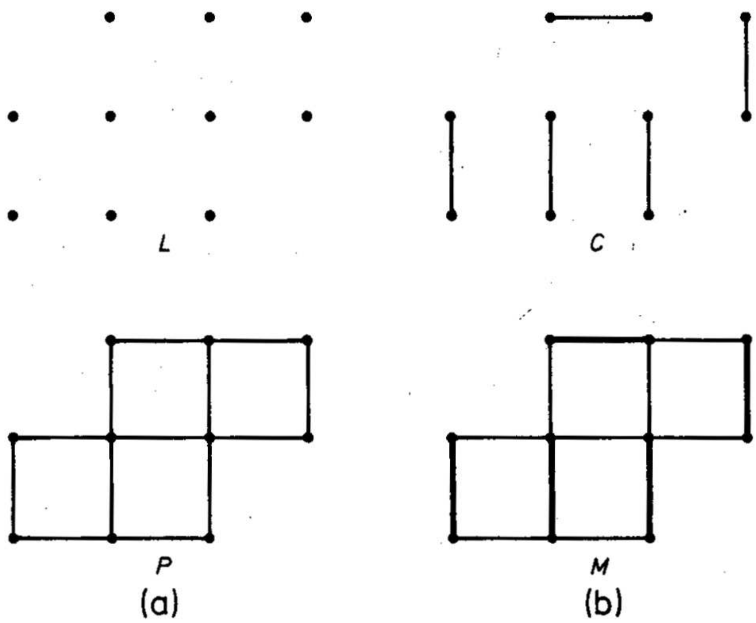


Fig. 1

A very similar question arose in the chemistry of benzenoid hydrocarbons. A *hexagonal system* (HS) is a connected finite plane graph with no cutpoints in which all interior regions are regular hexagons of side length one. An HS is the skeleton of some benzenoid hydrocarbon molecule if and only if it has a PM (Kekulé structure) (see, e.g., [7], [8], [12]). Given an HS, the chemist is interested in the number of all PMs as well as in the probability of finding a given edge in some PM (this probability is Pauling's bond order). It turned out that the methods developed for hexagonal systems (see [5]–[8]) can also be applied to polyominoes; however, some preparation is needed.

All graphs $G$ to be considered in the sequel are finite, multiple edges are allowed to occur. $V(G)$ denotes the set of vertices of $G$, and $n(G) = |V(G)|$.

**2. A basic theorem.** Let $G$ be a finite plane graph; $G$ subdivides the plane into a finite number $f$ of (connected, open) regions. A region $F$ is called a (2 mod 4)*-region* if the length $l(C)$ of every component $C$ of the boundary of $F$ satisfies

(1) $$l(C) \equiv 2 \pmod 4;$$

$G$ is called a (2 mod 4)-*graph* if all of its regions are (2 mod 4)-regions (Fig. 2).

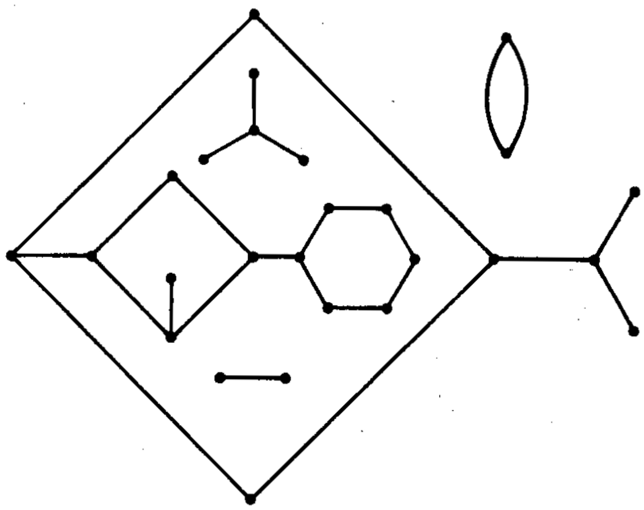

Fig. 2. A (2 mod 4)-graph

The following theorem (see [13] and [14]) generalizes a result of Cvetković et al. [2] (see also [3] and [1], 8.2); it follows also from a more general theorem of Kasteleyn expressing the number of perfect matchings of a plane graph in terms of a Pfaffian (see [9]).

THEOREM 1. *Let $G$ be a* (2 mod 4)-*graph with adjacency matrix $A$ which has $n$ vertices and let $m$ denote the number of perfect matchings contained in $G$. Then*

(A) *$n$ is even,*

(B) *$G$ is bipartite,*

(C) $\det A = (-1)^h m^2$, *where $h = n/2$.*

We need also

THEOREM 2. *Let $G$ be a connected plane graph whose interior regions are all* (2 mod 4)-*regions. Then $G$ is a* (2 mod 4)-*graph if and only if it has an even number of vertices.*

Proof. Let $F_0, F_1, \ldots, F_{f-1}$ be the regions of $G$, where $F_0$ is the exterior (infinite) region, and let $l_i$ denote the length of the boundary of $F_i$. We have to show that $l_0 \equiv 2 \pmod 4$ if and only if $n = n(G)$ is even. Let $k$ be the number of edges of $G$. Clearly,

$$2k = l_0 + l_1 + \ldots + l_{f-1} \equiv l_0 + (f-1)\cdot 2 \pmod 4.$$

By Euler's polyhedron formula, $2k = 2n + 2f - 4$. Thus $l_0 \equiv 2n + 2 \pmod 4$.

**3. Trapezoidal systems.** Let $P$ be a polyomino over a square lattice. Fix a vertex $z$ of $P$ and colour it black; colour all vertices of $P$ black and white so that every edge connects a black vertex with a white one. Lift the white vertices and pull the black ones down by 1/4 each thus transforming $P$ into a *trapezoidal system* $T = T(P)$ (Fig. 3). By this operation the set of edges is partitioned into three classes: long (vertical), short (vertical), and oblique. Subdivide every long edge by inserting two additional vertices (a black one and a white one) so that the three new edges are of length 1/2 each, as indicated in Fig. 3. By these operations, $P$ is transformed into an "extended trapezoidal system" $T' = T'(P)$ in which, with respect to the lowest white vertices (which define the zero level), every vertex $x$ has a well-defined height $h(x)$ (Fig. 3).

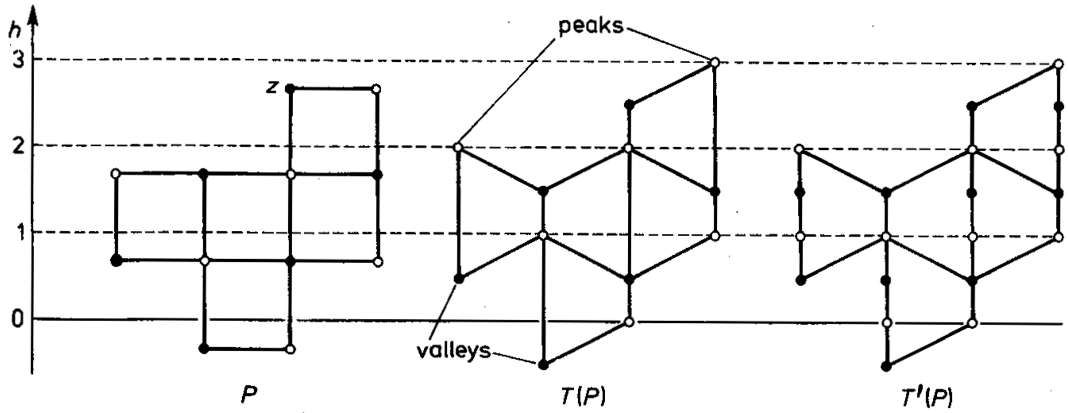


Fig. 3

A white vertex $x_0$ (black vertex $y_0$) whose neighbours are all lower than $x_0$ (higher than $y_0$) is called a *peak* (*valley*). Let $w$, $b$, $p$, $v$ be the numbers of white vertices, black vertices, peaks, and valleys of $T(P)$, respectively, and let $w'$, $b'$, $p'$, $v'$ have the analogous meanings with respect to $T'(G)$.

Observation 1. *The peaks and valleys are precisely those vertices which, in $T(P)$, are not incident with a short edge.*

Since the short edges are disjoint and every short edge connects a white vertex with a black one, we conclude that

$$p - v = w - b. \tag{2}$$

Clearly, $p' = p$, $v' = v$, and $w' - b' = w - b$, so

$$p' - v' = w' - b'. \tag{2'}$$

Observation 2. *The PMs of $P$ are in a* (1, 1)*-correspondence with the PMs of $T(P)$ as well as $T'(P)$; therefore,*

$$m(P) = m(T(P)) = m(T'(P)) \tag{3}$$

(Fig. 4).

Let $n = n(P)$ and $n' = n(T'(P))$; clearly, $n' \equiv n \pmod 2$.

Observation 3. *If $n$ is even, then* (by Theorem 2) *$T'(P)$ is a* (2 mod 4)*-graph; therefore* (according to Theorem 1 (C) and Observation 2)

$$m^2 = |\det A'|, \tag{4}$$

*where $m = m(P)$ and $A'$ is the adjacency matrix of $T'(P)$.*

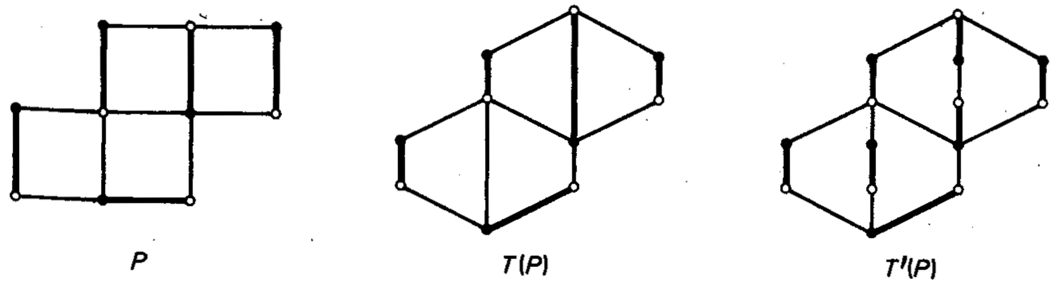


Fig. 4

It will be our main concern to derive from (4) a simple determinant formula for $m$ where the size of the matrix is considerably reduced as compared with the size of $A'$ or $A$.

Let $S^*$ denote the set of all connected graphs which are subgraphs of some polyomino.

OBSERVATION 4. *The transformations $T$ and $T'$ described above can be applied analogously to any graph $G \in S^*$ transforming $G$ into $T(G)$ and $T'(G)$, respectively, and the statements made in Observations* 1 *and* 2 *remain valid for $G$; the analogue of formula* (4) *is also true for $G$ provided $T'(G)$ is a* (2 mod 4)-*graph.*

Let $Z$ denote the set of all (2 mod 4)-graphs and put

$$S = \{G | \ G \in S^* \text{ and } T'(G) \in Z\}.$$

Next two simple characterizations of the members of $S$ shall be given.

Let $F$ be an interior region of a graph $G \in S^*$ and let $i(F)$ denote the number of lattice points lying in the interior of $F$ (Fig. 5).

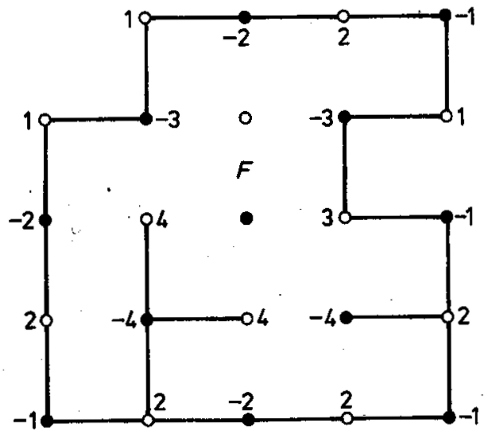


Fig. 5

$i(F) = 2, \ h(F) = 0$

LEMMA 1. *$T'(F)$ is a* (2 mod 4)-*region if and only if $i(F)$ is even.*

This can be proved by induction on the number of cells covered by $F$.

Let $X(F)$ denote the set of vertices lying on the boundary of $F$. Let $x \in X(F)$ and let the total measure of the (open) angles which have their vertex at $x$ and are open towards the interior of $F$ be $k_F(x)\cdot\pi/2$ ($k_F(x)\in\{1, 2, 3, 4\}$). Put

$$\operatorname{sgn}(x) = \begin{cases} 1 & \text{if } x \text{ is white,} \\ -1 & \text{if } x \text{ is black} \end{cases}$$

and

$$\hat{h}(F) = \left|\frac{1}{4}\sum_{x\in X(F)} \operatorname{sgn}(x)\cdot k_F(x)\right|$$

(Fig. 5).

LEMMA 2. *For each interior region $F$ of a graph $G\in S^*$, $\hat{h}(F)$ is an integer. $T'(F)$ is a* (2 mod 4)*-region if and only if $\hat{h}(F)$ is even.*

Again, the proof can be carried out by induction on the number of cells covered by $F$, making use of Lemma 1.

From these lemmata and Theorem 2 we obtain

THEOREM 3. *For a graph $G\in S^*$ the following statements are equivalent:*

(i) $G\in S$.

(ii) $n(G)$ *is even and* $i(F)$ *is even for every interior region* $F$ *of* $G$.

(iii) $n(G)$ *is even and* $\hat{h}(F)$ *is even for every interior region* $F$ *of* $G$.

COROLLARY 1. *Whether or not a graph $G\in S^*$ is a member of $S$ does neither depend on the choice of the distinguished vertex $z$ (the colours may be interchanged) nor on the position of $G$ in the plane ($G$ may be turned by multiples of* 90°).

COROLLARY 2. *Let $G\in S$.*

*Let $e$ be an edge of $G$ such that $G-e$ is connected; then $G-e\in S$.*

*Let $G'$ be a connected subgraph of $G$ with an even number of vertices such that $G'':=G-V(G')$ is connected; then $G'\in S$ and $G''\in S$.*

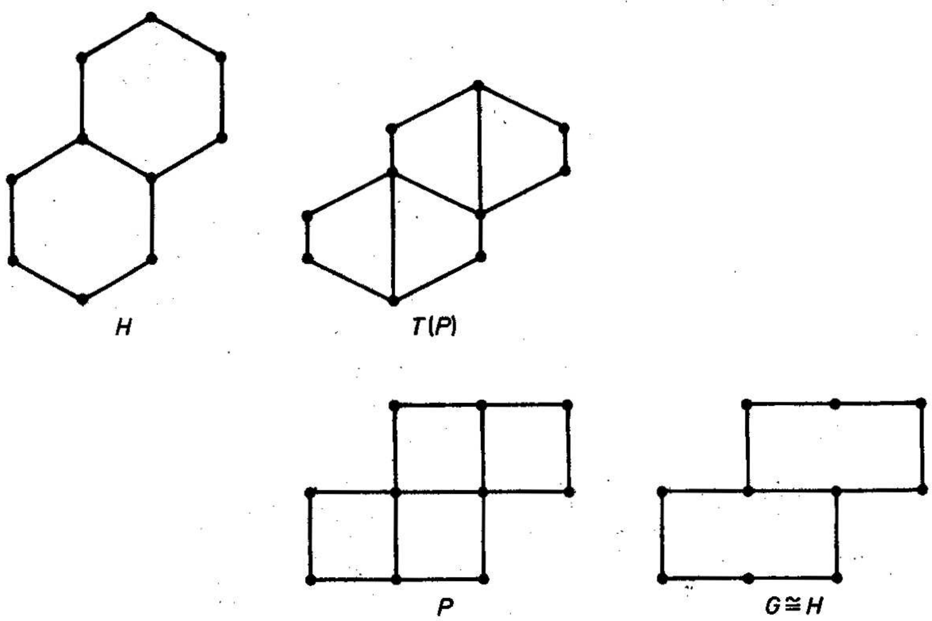


Fig. 6

COROLLARY 3. *Any hexagonal system $H$ can be obtained from some polyomino $P$ by deleting all long edges of $T(P)$* (Fig. 6); *thus the hexagonal systems which have an even number of vertices may be considered members of* $S$. *This implies that the entire theory to be developed for the members of $S$ is a fortiori valid for hexagonal systems with an even number of vertices.*

**4. Perfect matchings and perfect path systems.** Let $G \in S$ and consider $T(G)$ and $T'(G)$. A *pv-path* is a path starting at a peak and running monotonically down to a valley. A *path system* is a set of pairwise disjoint pv-paths; it is called *perfect* if every peak and every valley is contained in some path of the system. Clearly, a necessary condition for a perfect path system (PPS) to exist is that the number of peaks equals the number of valleys, i.e., $p = v$ or, equivalently (by Observation 1), $w = b$ or $w' = b'$, respectively. Evidently, the same condition is necessary for a PM to exist.

Suppose that $G$ has a PM. Let $M$ be any PM of $T(G)$; colour the edges of $M$ red and the others blue. It is not difficult to see that the long and the oblique edges which are red together with the short edges which are blue form a PPS, say $Q =: f(M)$. Conversely: Assume that $T(G)$ has a PPS. Let $Q$ be a PPS of $T(G)$; first colouring the short edges red and all others blue and then interchanging the colours of all edges that lie on some path of $Q$ results in a PM, say $M =: g(Q)$. It is almost evident that $g$ is the inverse of $f$, i.e., $Q = f(M)$ implies $M = g(Q)$, and conversely (Fig. 7).

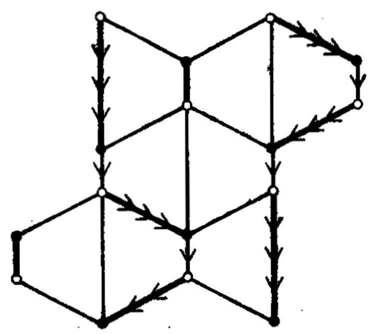

Fig. 7

Thus a (1, 1)-correspondence between the set of PMs (of $G$, $T(G)$ or $T'(G)$) and the set of PPSs (of $T(G)$ or $T'(G)$) (these sets may be empty) is established, in particular, the number $q = q(T(G)) = q(T'(G))$ of PPSs is equal to the number $m = m(G) = m(T(G)) = m(T'(G))$ of PMs:

THEOREM 4. *Let $G \in S^*$. There is a simple (1, 1)-correspondence between the set of perfect matchings of $G$ (or $T(G)$ or $T'(G)$) and the set of perfect path systems of $T(G)$ (or $T'(G)$) implying*

$$m(G) = q(T(G)) = q(T'(G)). \tag{5}$$

**5. The main theorem.** Let $G \in S^*$ and assume that $w = b$ implying, by Observations 4 and 1, $p' = p = v' = v$. Let

$$X_p = \{x_1, x_2, \ldots, x_p\} \quad \text{and} \quad Y_v = \{y_1, y_2, \ldots, y_p\}$$

be the sets of the peaks and the valleys, respectively, of $T(G)$ or of $T'(G)$ (which, without danger of confusion, can be identified) and let $q_{ik}$ denote the number of pv-paths connecting $x_k$ with $y_i$ $(1 \leqslant i, k \leqslant p)$; clearly, these numbers are the same for $T(G)$ and $T'(G)$. Put $Q := (q_{ik})$.

THEOREM 5. *For any graph $G \in S$ with as many black vertices as white ones,*

$$m(G) = q(T(G)) = |\det Q|. \tag{6}$$

As to the efficiency of Theorem 5, it is important to note that the numbers $q_{ik}$ can be very easily calculated. Let $x$ be any vertex of $T(G)$ or $T'(G)$, let $q_k(x)$ denote the number of monotone paths issuing from the peak $x_k$ and terminating at $x$ $(k = 1, 2, \ldots, p)$, put

$$\boldsymbol{q}(x) := (q_1(x), q_2(x), \ldots, q_p(x));$$

clearly, $q_k(y_i) = q_{ik}$ $(i = 1, 2, \ldots, p)$ and

$$Q = (q_{ik}) = \begin{bmatrix} \boldsymbol{q}(y_1) \\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ \boldsymbol{q}(y_p) \end{bmatrix}. \tag{7}$$

Let $U(x)$ denote the "upper neighbourhood" of $x$, i.e., the set of neighbours $x'$ of $x$ satisfying $h(x') > h(x)$. In order to calculate the vectors $\boldsymbol{q}(x)$, note simply the following:

(i) For any peak $x_k$,

$$\boldsymbol{q}(x_k) = (\delta_{k1}, \delta_{k2}, \ldots, \delta_{kp}),$$

where $\delta_{ii} = 1$, $\delta_{ij} = 0$ if $i \neq j$ $(k = 1, 2, \ldots, p)$.

(ii) For any vertex $x$ which is not a peak,

$$\boldsymbol{q}(x) = \sum_{x' \in U(x)} \boldsymbol{q}(x') \tag{8}$$

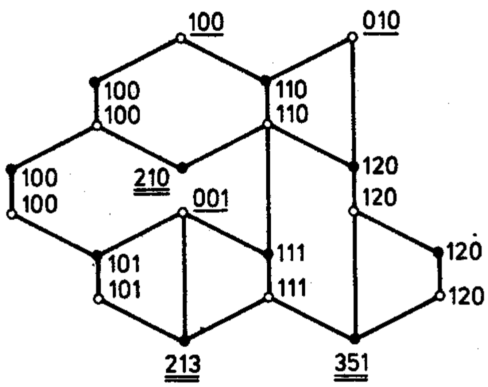


Fig. 8

(especially, $q(x) = 0$ if $x$ is a black vertex which has no upper neighbours). Running through $G$ from top to bottom, the $q(x)$ can now be successively determined. See Fig. 8, where

$$Q = \begin{bmatrix} 2 & 1 & 0 \\ 2 & 1 & 3 \\ 3 & 5 & 1 \end{bmatrix}.$$

**6. Proof of Theorem 5.** Let $G$ be as in Theorem 5 and consider $T'(G)$: by Observations 4 and 1, $w' = b'$. Let

$$X' = \{x_1, x_2, \dots, x_{w'}\}$$

and

$$Y' = \{y_1, y_2, \dots, y_{w'}\} = \{x_{w'+1}, x_{w'+2}, \dots, x_{n'}\}$$

(where $y_i = x_{w'+i}$) be the sets of the white and the black vertices, respectively, where (as above) $x_1, x_2, \dots, x_p$ are the peaks and $y_1, y_2, \dots, y_p$ are the valleys. The adjacency matrix of $T'(G)$ then takes the form

$$A' = \begin{bmatrix} O & B'^{\mathrm{T}} \\ B' & O \end{bmatrix},$$

and from Observations 2–4 and Theorem 4 we obtain

(9) $$m(G) = q(T(G)) = m(T'(G)) = |\det B'|.$$

We have to show that $|\det B'| = |\det Q|$. This will be performed by applying a simple Gaussian elimination process (in a more or less disguised form) to $\det B'$ reducing it to $\pm\det Q$.

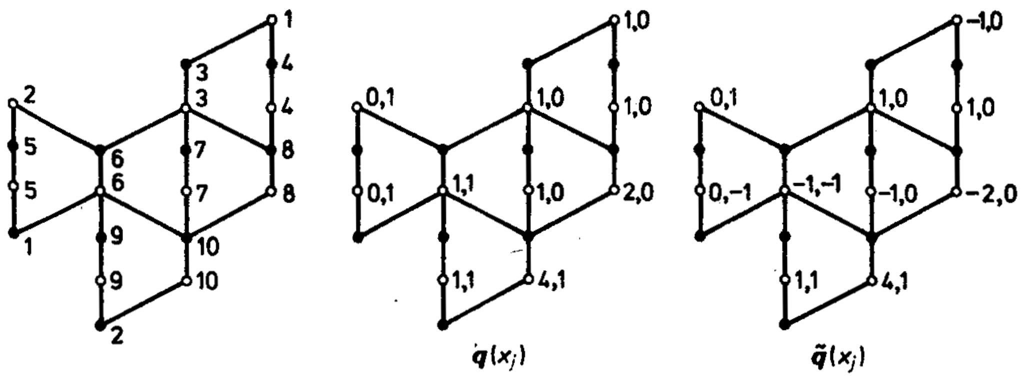


Fig. 9 (see also Fig. 3)

We may assume that the vertices are numbered as follows (Fig. 9):

(i) numbers $1, 2, \dots, p$ are reserved for the peaks and valleys;

(ii) any white vertex which is not a peak is given a number

$$j \in \{p+1, p+2, \dots, w'\}$$

such that $h(x_i) > h(x_k)$ implies $i < k$ $(i, k \in \{p+1, p+2, \dots, w'\})$;

(iii) every black vertex which is not a valley is given the same number as its unique lower neighbour.

Then $B'$ takes the form

$$B' = \begin{array}{cc} \begin{bmatrix} C & U \\ V & D \end{bmatrix} & \begin{array}{c} p \\ d \end{array} \\ \begin{array}{cc} p & d \end{array} & \end{array}, \tag{10}$$

where $d = w' - p$ and $D = (d_{ik}) = (b'_{p+i,p+k})$ $(i, k = 1, 2, \ldots, d)$ is a triangular matrix satisfying $d_{ik} = 0$ if $i < k$, $d_{ii} = 1$. Thus

$$\det D = 1. \tag{I}$$

Put

$$[C \quad U] =: R \quad \text{and} \quad [V \quad D] =: S; \tag{11}$$

so, by (10),

$$B' = \begin{bmatrix} R \\ S \end{bmatrix}. \tag{12}$$

Let $I_s$ denote the $s \times s$ unit matrix. Clearly,

$$[\boldsymbol{q}^{\mathrm{T}}(x_1), \boldsymbol{q}^{\mathrm{T}}(x_2), \ldots, \boldsymbol{q}^{\mathrm{T}}(x_p)] = I_p.$$

Put

$$[\boldsymbol{q}^{\mathrm{T}}(x_{p+1}), \boldsymbol{q}^{\mathrm{T}}(x_{p+2}), \ldots, \boldsymbol{q}^{\mathrm{T}}(x_{w'})] =: F,$$

$$[I_p \quad F] = [\boldsymbol{q}^{\mathrm{T}}(x_1), \boldsymbol{q}^{\mathrm{T}}(x_2), \ldots, \boldsymbol{q}^{\mathrm{T}}(x_{w'})] =: H;$$

put, further,

$$(-1)^{h(x_j)} \boldsymbol{q}(x_j) =: \tilde{\boldsymbol{q}}(x_j) \quad (j = 1, 2, \ldots, w') \tag{13}$$

(Fig. 9),

$$[\tilde{\boldsymbol{q}}^{\mathrm{T}}(x_1), \tilde{\boldsymbol{q}}^{\mathrm{T}}(x_2), \ldots, \tilde{\boldsymbol{q}}^{\mathrm{T}}(x_p)] =: \tilde{I}_p,$$

$$[\tilde{\boldsymbol{q}}^{\mathrm{T}}(x_{p+1}), \tilde{\boldsymbol{q}}^{\mathrm{T}}(x_{p+2}), \ldots, \tilde{\boldsymbol{q}}^{\mathrm{T}}(x_{w'})] =: \tilde{F},$$

$$[\tilde{I}_p \quad \tilde{F}] =: \tilde{H}, \quad [\underset{p}{O} \quad I_d] =: \tilde{K}$$

and

$$\begin{bmatrix} \tilde{I}_p^{\mathrm{T}} & O \\ \tilde{F}^{\mathrm{T}} & I_d \end{bmatrix} = [\tilde{H}^{\mathrm{T}} \quad \tilde{K}^{\mathrm{T}}] =: Z; \tag{14}$$

note that

$$|\det Z| = |\det \tilde{I}_p| \cdot |\det I_d| = 1. \tag{II}$$

The $(p \times w')$-matrix $R$ (see (11)) reflects the neighbourhoods of the valleys; therefore, because of (8),

$$RH^{\mathrm{T}} = Q = [q^{\mathrm{T}}(y_1), q^{\mathrm{T}}(y_2), \ldots, q^{\mathrm{T}}(y_p)]^{\mathrm{T}}$$

(see (7)). Put

(15) $$R\tilde{H}^{\mathrm{T}} =: \tilde{Q} =: [\tilde{q}_1^{\mathrm{T}}, \tilde{q}_2^{\mathrm{T}}, \ldots, \tilde{q}_p^{\mathrm{T}}]^{\mathrm{T}}$$

and note that the $i$-th row $\tilde{q}_i$ of $\tilde{Q}$ is either equal to the $i$-th row $q(y_i)$ of $Q$ or differs from it only by the factor $-1$ (in fact, because of (13) we have $\tilde{q}_i = (-1)^{h(y_i)+1/2}\, q(y_i)$); thus

(III) $$|\det \tilde{Q}| = |\det Q|.$$

The $(d \times w')$-matrix $S = [V \quad D]$ (see (11)) reflects the neighbourhoods of those black vertices which are not valleys; therefore, by (8) and (13),

(16) $$S\tilde{H}^{\mathrm{T}} = O.$$

Further,

(17) $$R\tilde{K}^{\mathrm{T}} = [C \quad U]\begin{bmatrix} O \\ I_d \end{bmatrix} = U,$$

(18) $$S\tilde{K}^{\mathrm{T}} = [V \quad D]\begin{bmatrix} O \\ I_d \end{bmatrix} = D.$$

Equations (12) and (14)–(18) yield

(19) $$B'Z = \begin{bmatrix} R \\ S \end{bmatrix}[\tilde{H}^{\mathrm{T}} \quad \tilde{K}^{\mathrm{T}}] = \begin{bmatrix} \tilde{Q} & U \\ O & D \end{bmatrix};$$

thus

(IV) $$\det(B'Z) = (\det \tilde{Q})(\det D).$$

From (II), (IV), (I), and (III) we now obtain in order

$$\begin{aligned} |\det B'| &= |\det B'| \cdot |\det Z| = |\det(B'Z)| \\ &= |\det \tilde{Q}| \cdot |\det D| = |\det \tilde{Q}| = |\det Q|. \end{aligned}$$

This proves the theorem.

**7. An example.** In how many ways can a $5 \times 6$ "chess-board" be covered by 15 dominoes such that each domino covers exactly two fields and each field is covered (by exactly one domino)? The answer is given by Fig. 10, where

$$Q = \begin{bmatrix} 52 & 39 \\ 39 & 52 \end{bmatrix} \quad \text{and} \quad m = |\det Q| = 1183.$$

More about covering chess-boards by dominoes in our "Problem" (see the Problems Section of this issue).

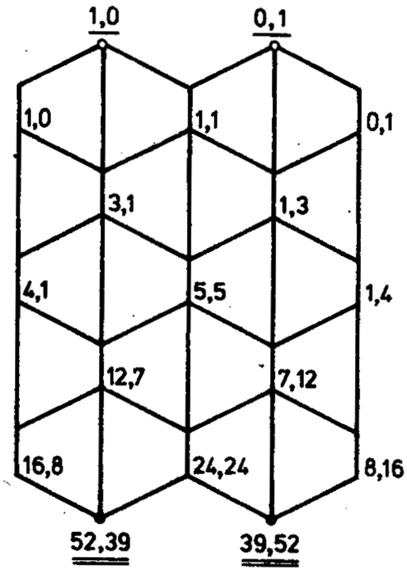


Fig. 10

**8. A different approach.** We have proved

(i) $$q(T(G)) = m(G) \quad \text{(Theorem 4)}$$

and

(ii) $$m(G) = |\det Q| \quad \text{(Theorem 5)}$$

implying

(iii) $$q(T(G)) = |\det Q| \quad \text{(Theorem 5)}.$$

For (i) we found a simple, intuitive combinatorial proof whereas (ii) was a bit harder. Comparing (i), (ii), and (iii), one is led to try to eliminate the concept of a perfect matching altogether by directly proving (iii), since this is a sort of an inclusion-exclusion principle for paths and path systems that has nothing to do with perfect matchings, and then to obtain (ii) from (i) and (iii) very easily – indeed, a plausible and challenging idea. However, there are some obstacles. That this program can nevertheless be carried through is shown in all details by Gronau et al. [5] who found a general determinant formula, discussed under what conditions it is valid, and applied it to hexagonal systems.

## References

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