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BOUNDS FOR THE NUMBER OF PERFECT MATCHINGS IN HEXAGONAL SYSTEMS

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Abstract. Upper bounds for the number of perfect matchings in hexagonal systems are deduced, which depend on the number of vertices and edges. The results are obtained using graph spectral theory.

A hexagonal unit cell is a plane region bounded by a regular hexagon. A hexagonal system is a finite connected plane graph with no cut-vertices in which every interior region is a hexagonal unit cell. A perfect matching of a hexagonal system H is a set of (disjoint edges of H which cover all vertices of H).

Perfect matchings in hexagonal systems have been studied in a number of recent publications [6–11]. In addition to this, both perfect matchings and hexagonal systems play an important role in theoretical chemistry [5] and there are numerous chemical papers concerned with this matter (for review and further references see [4, 5]).

The number of vertices edges and perfect matchings of a hexagonal system H will be denoted by n, m and k, respectively. An obvious necessary condition for the existence of perfect matchings in a graph is that the number of its vertices is even Therefore throughout this paper we shall assume that n is an even number. It is clear that in hexagonal systems n cannot be less than 6 and we shall often need the fact that $n/2 - 2 > 0$.

The adjacency matrix A of H is a square matrix of order n whose rs entry is equal to 1 if the vertices r and s of H are adjacent and is otherwise equal to 0. The eigenvalues of A are called the eigenvalues of H. Let $X_1, X_2, \dots, X_n$ be the eigenvalue of H, labeled so that $X_i \geq X_j$ for $i < j$.

For any graph with m edges [1],

$$\textstyle\sum_{i=1}^{n} X_i^2 = 2m$$

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whereas for any bipartite graph $X_i = -X_{n-i+1}$, $i = 1, 2, \ldots, n$.

Since hexagonal systems are bipartite graphs, we immediately deduce that

$$\sum_{i=1}^{n/2} X_i^2 = m \tag{1}$$

For hexagonal systems two further relations for the graph eigenvalues hold, viz.:

$$\sum_{i=1}^{n/2} X_i^4 = 9m - 6n \tag{2}$$

and

$$\prod_{i=1}^{n/2} X_i = k \tag{3}$$

Formula (2) is obtained in [3] whereas (3) is first reported in [2]. For a complete proof of (3) see pp. 242–243 of [1].

Consider now non-negative quantities $x_1, x_2, \ldots, x_{n/2}$ which satisfy the condition

$$\sum_{i=1}^{n/2} x_i^2 = m.$$

LEMMA 1. *If* $(1')$ *holds, then*

$$\prod_{i=1}^{n/2} x_i \leq (2m/n)^{n/4}.$$

Furthermore, equality in (4) *occurs if and only if* $x_1 = x_2 = \cdots = x_{n/2}$.

Proof. If some of the x_i's are equal to zero, then the inequality (4) holds in a trivial manner. Suppose therefore that all x_i's are positive and find the extreme of the functional L,

$$L = \sum_{i=1}^{n/2} \ln x_i.$$

under the constraint $(1')$. A straightforward use of standard variational calculus yields the condition

$$x_i^{-1} + 2\lambda x_i = 0$$

which must hold for all $i = 1, 2, \ldots, n/2$. From (6), $x_i = (-2\lambda)^{-1/2}$ and because of $(1')$, $x_i = (2m/n)^{1/2}$ for all $i = 1, 2, \ldots, n/2$.

Lemma 1 follows now immediately. □

Bearing in mind the analogy between eqs. (1) and $(1')$ as well as between the l.h.s. of (3) and (4), we arrive at the following conclusion.

THEOREM 1. *For all hexagonal systems with* n *vertices,* m *edges and* k *perfect matchings*

$$k < (2m/n)^{n/4}. \tag{7}$$

Let us consider now a somewhat more complicated problem and seek for the extremes of the functional $\prod_{i=1}^{n/2} x_i$ under the constraint $(1')$ and

$$\sum_{i=1}^{n/2} x_i^4 = 9m - 6n. \tag{2'}$$

Here again we may focus our attention on the case when all x_i's are positive. A reasoning fully analogous to that used in the proof of Lemma 1 leads to the condition.

$$x_i^{-1} + 2\lambda x_i + 4\mu x_i^3 = 0 \tag{8}$$

which must be satisfied for all $i = 1, 2, \ldots, n/2$. Equation (8) is transformed into

$$1 + 2\lambda x_i^2 + 4\mu x_i^4 = 0. \tag{9}$$

Whatever is the value of the Lagrange multipliers λ and μ, equation (9) has either two positive roots or no real root. From the analysis which follows it will be seen that (9) has real roots in some cases of interest for the present consideration.

Suppose that A and B are positive real roots of (9), $A > B > 0$. Then some of the x_i's will be equal to A and the rest of them will be equal to B. Because of Lemma 1 we must not choose all the x_i's to be mutually equal.

Let therefore t among the x_i's be equal to A, $1 \leq t \leq n/2 - 1$. Let, in particular, in the case when $t = 1$,

$$x_{n/2-1} = A, \quad x_1 = \cdots = x_{n/2-2} = B, \quad x_{n/2} = B. \tag{10a}$$

in the case when $t = n/2 - 1$,

$$x_1 = \cdots = x_{n/2-1} = A, \quad x_{n/2} = B \tag{10b}$$

and in the case when $1 < t < n/2 - 1$,

$$x_1 = \cdots = x_{t-1} = A, \quad x_{n/2-1} = A, \quad x_t = \cdots = x_{n/2-2} = B, \quad x_{n/2} = B. \tag{10c}$$

The reason for such an unusual assignment will become clear later.

Substituting any of the relations (10) back into $(1')$ and $(2')$, we obtain

$$tA^2 + (n/2 - t)B^2 = m, \quad tA^4 + (n/2 - t)B^4 = 9m - 6n \tag{11}$$

from which

$$A = A(t) = (2m/n + RS)^{1/2}, \qquad B = B(t) = (2m/n - R/S)^{1/2} \tag{12}$$

where

$$R = (18mn - 12n^2 - 4m^2)^{1/2} n^{-1}, \qquad S = [(n - 2t)/(2t)]^{1/2}. \tag{13}$$

LEMMA 9. *For all values of the parameters n and m which can occur in hexagonal systems, $18mn - 12n^2 - 4m^2 > 0$.*

Proof. It is easily seen that $18mn - 12n^2 - 4m^2$ is positive if

$$(9 - \sqrt{33})n/4 < m < (9 + \sqrt{33})n/4, \quad \text{i.e.} \quad 1.6 < 2m/n < 7.4. \tag{14}$$

Now $2m/n$ is the average vertex degree of the hexagonal system considered. Obviously, for all hexagonal systems $2m/n$ lies between 2 and 3 and therefore the inequalities (14) are certainly fulfilled. □

As a consequence of Lemma 2, R, as defined in (13), is necessarily real. Therefore $A(t)$ is real for all t, $0 < t < n/2$ whereas $B(t)$ is real for $0 < t \leq m^2/(9m - 6n)$.

If the x_i's are chosen according to (10), then the functional L, in (5), becomes equal to $L(t)$:

$$L(t) = t \ln A + (n/2 - t) \ln B \tag{15}$$

with A and B given by equations (12).

LEMMA. *Provided A and B are real (i.e. for $0 < t \leq m^2/(9m - 6n)$) $L(t)$ is a monotonously decreasing function of the parameter t.*

Proof. Differentiate equations (11) with respect to t

$$A^2 + 2tAA' - B^2 + 2(n/2 - t)BB' = 0$$
$$A^4 + 4tA^3A' - B^4 + 4(n/2 - t)B^3B' = 0$$

and calculate A' and B' as

$$A' = -(A^2 - B^2)/(4tA), \qquad B' = -(A^2 - B^2)/(2nB - 4tB). \tag{16}$$

From (15) we get

$$L'(t) = \ln A + tA'/A - \ln B + (n/2 - t)B'/B$$

which combined with (16) gives

$$L'(t) = \ln(A/B) - (A/B)^2/4 + (A/B)^{-2}/4.$$

For $A > B$, $L'(t)$ is negative. In order to see this, notice that if $f(x) = \ln x - x^2/4 + x^{-2}/4$, then $f(1) = 0$ and $f'(x) = -(x^2 - 1)^2/(2x^3)$. Hence for $x > 1$, $f(x) < 0$. □

For $t = 1, 2, \ldots, [m^2/(9m - 6n)]$, $L(t)$ is a stationary point if the functional L, equation (5). From Lemma 3 one may expect that for $t = 1$, $L(t)$ is a maximum. We now show that this is indeed the case.

The quantities $x_1, x_2, \ldots, x_{n/2}$ can be understood as variables which are to be determined by variational calculus. Because of (1′) and (2′), only $n/2 - 2$ of them are independent. Let these be $x_1, x_2, \ldots, x_{n/2-2}$ and denote the dependent variables $x_{n/2-1}$ and $x_{n/2}$ by y and z, respectively. (Note that in all the relations (10) $y = A$ and $z = B$.)

Let $f(x)$ be an arbitrary function of x, such that $f(x)$ and its first and second derivatives exit for $x = x_i$, $i = 1, 2, \ldots, n/2$. Consider a functional F,

$$F = F(x_1, x_2, \ldots, x_{n/2-2}) = \textstyle\sum_{i=1}^{n/2} f(x_i).$$

Then for $i, j = 1, 2, \ldots, n/2-2$,

$$\frac{\partial F}{\partial x_i} = f'(x_i) + \frac{\partial y}{\partial x_i} f'(y) + \frac{\partial z}{\partial x_i} f'(z) \tag{17}$$

$$\begin{aligned}\frac{\partial^2 F}{\partial x_i \partial x_j} &= \delta_{ij} f''(x_i) + \frac{\partial^2 y}{\partial x_i \partial x_j} f'(y) + \frac{\partial y}{\partial x_j}\,\frac{\partial y}{\partial x_j} f''(y) \\ &+ \frac{\partial^2 z}{\partial x_i \partial x_j} f'(z) + \frac{\partial z}{\partial x_i}\,\frac{\partial z}{\partial x_j} f''(z)\end{aligned} \tag{18}$$

where $\delta_{ii} = 1$ and $\delta_{ij} = 0$ for $i \neq j$. As special case of (17) and (18) we get from (1′) and (2′):

$$x_i + y\frac{\partial y}{\partial x_i} + z\frac{\partial z}{\partial x_i} = 0, \qquad x_i^3 + y^3\frac{\partial y}{\partial x_i} + z^3\frac{\partial z}{\partial x_i} = 0 \tag{19}$$

$$\delta_{ij} + y\frac{\partial^2 y}{\partial x_i\,\partial x_j} + \frac{\partial y}{\partial x_i}\,\frac{\partial y}{\partial x_j} + z\frac{\partial^2 z}{\partial x_i\,\partial x_j} + \frac{\partial z}{\partial x_i}\,\frac{\partial z}{\partial x_j} = 0 \tag{20}$$

$$3\delta_{ij}x_i^2 + y^3\frac{\partial^2 y}{\partial x_i\,\partial x_j} + 3y^2\frac{\partial y}{\partial x_i}\,\frac{\partial y}{\partial x_j} + z^3\frac{\partial^2 z}{\partial x_i\,\partial x_j} + 3z^2\frac{\partial z}{\partial x_i}\,\frac{\partial z}{\partial x_j} = 0. \tag{21}$$

In what follows we have distinguish between three cases: (a) $t = 1$, (b) $t = n/2-1$ and (c) $1 < t < n/2-1$. Since the examination is virtually the same in all the there cases, we shall consider here only case (c).

Thus let $1 < t < n/2-1$. Denote the sets $\{1, \ldots, t-1\}$ and $\{t, \ldots, n/2-2\}$ by I_A and I_B, respectively. In the case (c), equations (10c) hold and after substituting them into (19) we get for $i \in I_A$:

$$A(1 + \partial y/\partial x_i) + B\partial z/\partial x_i = 0, \qquad A^3(1 + \partial y/\partial x_i) + B^3\partial z/\partial x_i = 0$$

from which

$$\partial y/\partial x_i = -1; \qquad \partial z/\partial x_i = 0. \tag{22}$$

For $i \in I_B$,

$$A\,\partial y/\partial x_i + B(1 + \partial z/\partial x_i) = 0, \qquad A^3\,\partial y/\partial x_i + B^3(1 + \partial z/\partial x_i) = 0$$

and therefore

$$\partial y/\partial x_i = 0; \quad \partial z/\partial x_i = -1. \tag{23}$$

Both (22) and (23), substituted back into (17) imply $\partial F/\partial x_i = 0$.

Now, for $i = j \in I_A$ we get from (20) and (21):

$$\frac{\partial^2 y}{\partial x_i^2} = \frac{2B - 6A^2}{A^3 - AB^2}, \qquad \frac{\partial^2 z}{\partial x_i^2} = \frac{-4A^2}{B^3 - A^2 B}$$

which results in $\partial^2 F/\partial x_i^2 = 2u$ where

$$u = f''(A) + f'(A)\frac{B^2 - 3A^2}{A^3 - AB^2} - \frac{2A^2 f'(B)}{B^3 - A^2 B}. \tag{24}$$

Similarly, for $i, j \in I_A$, $i \neq j$, $\partial^2 F/\partial x_i\,\partial x_j = u$, for $i = j \in I_B$, $\partial^2 F/\partial x_i^2 = 2w$ where

$$w = f''(B) + f'(B)\frac{A^2 - 3B^2}{B^3 - A^2 B} - \frac{2B^2 f'(A)}{A^3 - AB^2} \tag{25}$$

for $i, j \in I_B$, $i \neq j$, $\partial^2 F/\partial x_i\,\partial x_j = w$ whereas for $i \in I_A$, $j \in I_B$ or $i \in I_B$, $j \in I_A$, $\partial^2 F/\partial x_i\,\partial x_j = 0$.

This means that the Hessian matrix of F has the block diagonal form

$$\begin{bmatrix} U & 0 \\ 0 & W \end{bmatrix},$$

where 0 is a zero matrix and

$$U = \begin{bmatrix} 2u & u & \dots & u \\ u & 2u & \dots & u \\ \vdots & \vdots & \ddots & \vdots \\ u & u & \dots & 2u \end{bmatrix}; \qquad W = \begin{bmatrix} 2w & w & \dots & w \\ w & 2w & \dots & w \\ \vdots & \vdots & \ddots & \vdots \\ w & w & \dots & 2w \end{bmatrix}.$$

Note that U and W are of order $t-1$ and $n/2-t-1$, respectively. Their eigenvalues are easily found. The eigenvalues of U are: u $(t-2)$-times and tu. The eigenvalues of W are: w $(n/2-t-2)$-times and $(n/2-t)w$.

In the problem we are concerned with, $f(x_i) = \ln x_i$, and then formulas (24) and (25) reduce to $u = -w = 2(A^2 - B^2)(AB)^{-2}$. Consequently, $u > 0$, $w < 0$ and we reach the following conclusion.

LEMMA 1. *The Hessian matrix of L, equation* (5), *has $t-1$ positive and $n/2-t-1$ negative eigenvalues.*

We have demonstrated the validity of Lemma 4 assuming that $1 < t < n/2-1$. The very same statement holds also in the case (a) $t = 1$ and (b) $t = n/2-1$. The proof of Lemma 4 in cases (a) and (b) is essentially the same as in the case (c) and will not be reproduced here. □

Since Lemma 4 holds for all t, $1 \leq t < n/2$, we arrive at our main results.

LEMMA 5. *$L(1)$ equation* (15), *is a maximum if and only if $t = 1$.*

LEMMA 6. *If* (1′) *and* (2′) *hold, then $\prod_{i=1}^{n/2} \leq K$, where*

$$K = (2m/n + R\sqrt{n/2-1})^{1/2}(2m/n - R/\sqrt{n/2-1})^{(n-2)/4} \tag{26}$$

and R is given by (13).

THEOREM 2. *For all hexagonal systems with n vertices, m edges and k perfect matching,*

$$k \leq K \tag{27}$$

with equality if and only if $n = 6$.

Proof. The main statement of Theorem 2 is an immediate consequence of Lemma 6. Only one hexagonal system, namely that composed of a single hexagon has only two distinct positive eigenvalues ($X_1 = 2, X_2 = X_3 = 1$). □

We demonstrate now that the upper bound given in Theorem 2 is better than the upper bound given in Theorem 1.

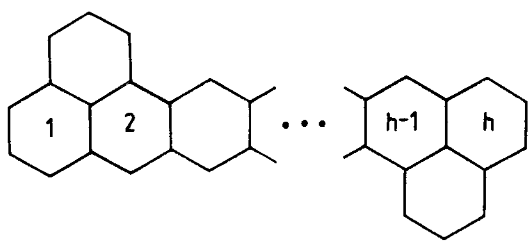
LEMMA 7. *For all values of the parameters* n *and* m *which may occur in hexagonal systems* $K < (2m/n)^{n/4}$.

Proof. Consider K, equation (26) as a function of the parameter R. Setting $R = 0$ into (26) one obtains just the upper bound from Theorem 1. Now,

$$\partial \ln K/\partial R = 1/2 \cdot \sqrt{n/2-1}[(2m/n + R\sqrt{n/2-1})^{-1} - (2m/n - R/\sqrt{n/2-1})^{-1}]$$

which for $R > 0$ is obviously negative. Hence $\ln K$ and thus also K is a decreasing function of R. According to Lemma 2, $R > 0$ for all combinations of n and m which occur in hexagonal systems. □

The upper bounds (7) and (27) both depend on n — the number of vertices and m — the number of edges. One may ask why our variational procedure did not result also in lower bounds for k.



As a matter of fact, lower bounds of this type probably cannot be found at all. Namely, whereas the parameters n and m increase with the increasing size of a hexagonal system, the number of perfect matchings need not do so. Even if we disregard hexagonal systems for which $k = 0$, there still remains an arbitrarily large number of examples for which $k < k_0$, where k_0 is a constant greater than 9. For instance, the following hexagonal system has 9 perfect matchings for all $h \geq 3$:

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