Summary of the Ph.D. dissertation

Graph Polynomials and Graph Transformations in Algebraic Graph Theory

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1. Introduction

In the center of the dissertation graph polynomials and graph transformations stand, their role in algebraic and extremal graph theoretic problems. The algebraic graph theory has a long history due to its intimate relationship with chemistry and (statistical) physics. In these fields one often describe a system, state or a molecule by an appropriate parameter. Then it rises the purely mathematical question whether what the extremal values of this parameter are. In the dissertation we give some general methods to attack these kinds of extremal problems. In the first, bigger half of the dissertation we study two graph transformations, the so-called Kelmans transformation and the generalized tree shift introduced by the author. The Kelmans transformation can be applied to all graphs, while one can apply the generalized tree shift only for trees. The importance of these transformations lies in the fact that surprisingly many natural graph parameters increase (or decrease) along these transformations. This way we gain a considerable information about the extremal values of the studied parameter.

In the second half of the dissertation we study a purely extremal graph theoretic problem, the so-called density Turán problem which, however, turn out to be strongly related to algebraic graph theory in several ways. As a by-product of the efforts we did to solve the problem we give a solution to a longstanding open problem concerning trees having only integer eigenvalues.

2. Notations and basic definitions

Before we start to survey our results, we introduce the most important notations.

We will follow the usual notation: G is a simple graph, $V(G)$ is the set of its vertices, $E(G)$ is the set of its edges. In general, $|V(G)| = n$ and $|E(G)| = e(G) = m$. We will use the notation $N(x)$ for the set of the neighbors of the vertex x, $|N(v_i)| = \deg(v_i) = d_i$ denote the degree of the vertex v_i. We will also use the notation $N[v]$ for the closed neighborhood $N(v) \cup \{v\}$. The complement of the graph G will be denoted by $\overline{G}$.

K_n will denote the complete graph on n vertices, meanwhile $K_{n,m}$ the complete bipartite graph with color classes of size n and m. Let P_n and S_n denote the path and the star on n vertices, respectively.

Let M_1 and M_2 be two graphs with distinguished vertices u_1, u_2 of M_1 and M_2, respectively. Let $M_1 : M_2$ be the graph obtained from M_1, M_2 by identifying the vertices of u_1 and u_2. So $|V(M_1 : M_2)| = |V(M_1)| + |V(M_2)| - 1$ and $E(M_1 : M_2) = E(M_1) \cup E(M_2)$. Note that this operation depends on the vertices u_1, u_2, but in general we do not indicate it in the notation.

The matrix $A(G)$ will denote the adjacency matrix of the graph G, i.e., $A(G)_{ij}$ is the number of edges going between the vertices v_i and v_j. Since $A(G)$ is symmetric, its eigenvalues are real and we will denote them by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. We will also use the notation $\mu(G)$ for the largest eigenvalue and we will call it the spectral radius of the graph G. The characteristic polynomial of the adjacency matrix will be denoted by

$$\phi(G, x) = \det(xI - A(G)) = \prod_{i=1}^{n} (x - \mu_i).$$

We will simply call it the adjacency polynomial.

The Laplacian matrix of G is $L(G) = D(G) - A(G)$ where $D(G)$ is the diagonal matrix for which $D(G)_{ii} = d_i$, the degree of the vertex v_i. We will denote the eigenvalues of the Laplacian matrix by $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_{n-1} \geq \lambda_n = 0$. The characteristic polynomial of the Laplacian matrix will be denoted by

$$L(G, x) = \det(xI - L(G)) = \prod_{i=1}^{n}(x - \lambda_i).$$

We will simply call it the Laplacian polynomial.

We mention here that $\tau(G)$ will denote the number of spanning trees of the graph G.

Let $m_r(G)$ denote the number of r independent edges (i.e., the r-matchings) in the graph G. We define the matching polynomial of G as

$$M(G, x) = \sum_{r=0}(-1)^r m_r(G)x^{n-2r}.$$

The roots of this polynomial are real, and we will denote the largest root by $t(G)$.

Let $i_k(G)$ denotes the number of independent sets of size k. The independence polynomial of the graph G is defined as

$$I(G, x) = 1 - i_1(G)x + i_2(G)x^2 - i_3(G)x^3 - \ldots$$

Let $\beta(G)$ denote the smallest real root of $I(G, x)$. It exists and it satisfies the inequality $0 < \beta(G) \leq 1$.

Let $ch(G, \lambda)$ be the chromatic polynomial of G; so for a positive integer λ the value $ch(G, \lambda)$ is the number of ways that G can be well-colored with λ colors. It is indeed a polynomial in λ and it can be written in the form

$$ch(G, x) = \sum_{k=1}^{n}(-1)^{n-k}c_k(G)x^k,$$

where $c_k(G) \geq 0$.

3. Kelmans transformation

We define the Kelmans transformation as follows.

Definition 3.1. Let u, v be two vertices of the graph G, we obtain the Kelmans transformation of G as follows: we erase all edges between v and $N(v)\backslash(N(u) \cup \{u\})$ and add all edges between u and $N(v)\backslash(N(u) \cup \{u\})$. The obtained graph has the same number of edges as G; in general we will denote it by G' without referring to the vertices u and v.

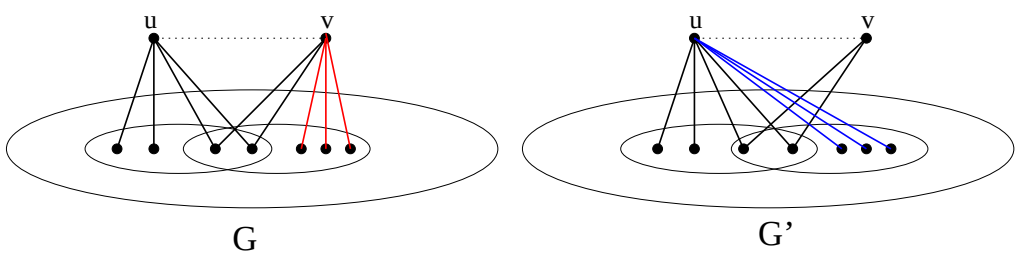

Figure 1. The Kelmans transformation.

Kelmans studied the following problem when he introduced his transformation. Let $R_q^k(G)$ be the probability that if we remove the edges of the graph G with probability q, independently of each other, then the obtained random graph has at most k components. Kelmans showed that the Kelmans transformation decreases this probability for every q, in other words, $R_q^k(G') \leq R_q^k(G)$. Satyanarayana, Schoppmann and Suffel [10] rediscovered this result and they proved that the Kelmans transformation decreases the number of spanning trees: $\tau(G') \leq \tau(G)$. We proved the following results.

Theorem 3.2. [1] *Let G' be obtained from G by a Kelmans transformation. Let $\mu(G)$ and $\mu(G')$ denote the largest eigenvalue of the adjacency matrix of G and G', respectively. Then $\mu(G') \geq \mu(G)$.*

This result enabled us to attain a breakthrough in an old problem of Eva Nosal. In this problem one has to bound the expression $\mu(G) + \mu(\overline{G})$ in terms of the number of vertices. We managed to prove the following theorem which was a significant improvement of the previous results.

Theorem 3.3. [1] *Let G be a graph on n vertices. Then*

$$\mu(G) + \mu(\overline{G}) \leq \frac{1+\sqrt{3}}{2} n.$$

We managed to prove the following theorems concerning graph polynomials.

Theorem 3.4. [5] *Let $M(G,x)$ be the matching polynomial of the graph G:*

$$M(G,x) = \sum_{r=0} (-1)^r m_r(G) x^{n-2r}.$$

Let $t(G)$ denote the largest root of the matching polynomial. Let G' be obtained from G by a Kelmans transformation.

Then $m_k(G') \leq m_k(G)$ holds for every $1 \leq k \leq n/2$ and $t(G') \geq t(G)$.

Theorem 3.5. [5] *Let $I(G,x)$ be the independence polynomial of the graph G:*

$$I(G,x) = \sum_{k=0} (-1)^k i_k(G) x^k.$$

Let $\beta(G)$ denote the smallest root of the independence polynomial. Let G' be obtained from G by a Kelmans transformation.

Then $i_k(G') \geq i_k(G)$ holds for every $1 \leq k \leq n$ and $\beta(G') \leq \beta(G)$.

Theorem 3.6. [5] *Let $L(G,x) = \sum_{k=1}^{n} (-1)^{n-k} a_k(G) x^k$ be the Laplacian polynomial of the graph G. Let G' be obtained from G by a Kelmans transformation.*

Then $a_k(G') \leq a_k(G)$ for $1 \leq k \leq n$.

Theorem 3.7. [5] *Let $ch(G,x) = \sum_{k=1}^{n} (-1)^{n-k} c_k(G) x^k$ be the chromatic polynomial of the graph G. Let G' be obtained from G by a Kelmans transformation.*

Then $c_k(G') \leq c_k(G)$ for $1 \leq k \leq n$.

4. Generalized tree shift

We define the generalized tree shift as follows.

Definition 4.1. [2] Let T be a tree and let x and y be vertices such that all the interior points of the path xPy (if they exist) have degree 2 in T. The *generalized tree shift* (GTS) of T is the tree T' obtained from T as follows: let z be the neighbor of y lying on the path xPy, let us erase all the edges between y and $N_T(y)\backslash\{z\}$ and add the edges between x and $N_T(y)\backslash\{z\}$. We will denote the obtained tree by T' without referring to the role of x and y. We call the generalized tree shift proper if T and T' are not isomorph.

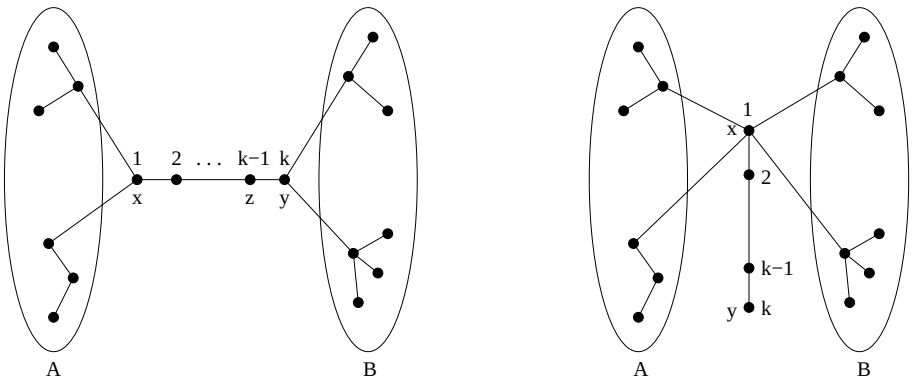

FIGURE 2. The generalized tree shift.

Notations: In what follows we assume that the path xPy has exactly k vertices. The set $A \subset V(T)$ consists of the vertices which can be reached with a path from k only through 1, and similarly the set $B \subset V(T)$ consists of those vertices which can be reached with a path from 1 only through k. Let H_1 be the tree induced by the vertices of $A \cup \{1\}$ in T, similarly let H_2 denote the tree induced by the vertices of $B \cup \{k\}$ in T. Note that H_1 and H_2 are both subtrees of T' as well.

This transformation determines a partially ordered set on the set of trees on n vertices.

Definition 4.2. [2] Let us say that $T' > T$ if T' can be obtained from T by some proper generalized tree shift. The relation $>$ induces a poset on the trees on n vertices, since the number of leaves of T' is greater than the number of leaves of T, more precisely the two numbers differ by one. Hence the relation $>$ is indeed extendable. We call this poset the induced poset of the generalized tree shift.

The following observation is very simple.

Theorem 4.3. [2] *The minimal element of the the induced poset of the generalized tree shift is the path on n vertices, its maximal element is the star on n vertices.*

Remark 4.4. So whenever we prove that the generalized tree shift increases a certain parameter we immediately obtain that the maximum of this parameter is attained at the star and the minimum of this parameter is attained at the path among the trees on n vertices.

In the sequel we survey some of the most important properties of the generalized tree shift.

Theorem 4.5. [2, 4] *Let T be a tree and let T' be obtained from T by a generalized tree shift.*

Then $m_k(T') \leq m_k(T)$ for $1 \leq k \leq n/2$. Furthermore, $\mu(T') \geq \mu(T)$ and $\mu(\overline{T'}) \geq \mu(\overline{T})$.

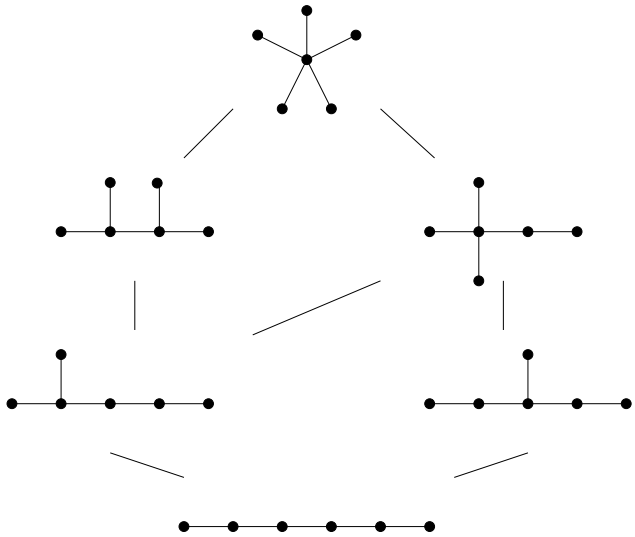

FIGURE 3. The poset of trees on 6 vertices.

Remark 4.6. In the case of trees the characteristic polynomial of the adjacency matrix and the matching polynomial coincide, in other words, $\phi(T,x) = M(T,x)$ and so $t(T) = \mu(T)$.

Theorem 4.7. [4] *Let $L(G,x) = \sum_{k=1}^{n}(-1)^{n-k}a_k(G)x^k$ be the Laplacian polynomial of the graph G. Let $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \lambda_{n-1}(G) \geq \lambda_n(G) = 0$ be the roots of $L(G,x)$, in other words, the eigenvalues of the Laplacian matrix. Let T be a tree and let T' be obtained from T by a generalized tree shift.*

Then $a_k(T') \leq a_k(T)$ for $1 \leq k \leq n$, $\lambda_1(T') \geq \lambda_1(T)$ and $\lambda_{n-1}(T') \geq \lambda_{n-1}(T)$.

Theorem 4.8. [4] *Let $I(G,x)$ be the independence polynomial of the graph G:*

$$I(G,x) = \sum_{k=0}(-1)^k i_k(G)x^k.$$

Let $\beta(G)$ denote the smallest root of the independence polynomial. Let T be a tree and let T' be obtained from T by a generalized tree shift.

Then $i_k(T') \geq i_k(T)$ for $1 \leq k \leq n$ and $\beta(T') \leq \beta(T)$.

Remark 4.9. There is a common thing in the above mentioned theorems, namely, all of the above mentioned graph polynomials satisfy a certain recursion formula. As a consequence one can factorize the expression $f(T',x) - f(T,x)$ in a special form. One can prove all the above mentioned theorem by this factorisation together with some "monotonicity" property of the studied parameter.

Lemma 4.10. [4] *Assume that the graph polynomials f and g satisfy the following recursion.*

$$f(M_1 : M_2, x) = c_1 f(M_1,x)f(M_2,x) + c_2 f(M_1,x)g(M_2|u_2,x) + \\ + c_2 g(M_1|u_1,x)f(M_2,x) + c_3 g(M_1|u_1,x)g(M_2|u_2,x),$$

where c_1, c_2, c_3 are rational functions of x. Furthermore, assume that $c_2 f(K_2) + c_3 g(K_2|1) \neq 0$. Then

$$f(T) - f(T') = c_4(c_2 f(P_k) + c_3 g(P_k|1))(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k)),$$

where

$$c_4 = \frac{g(P_3|1) - g(P_3|2)}{(c_2 f(K_2) + c_3 g(K_2|1))^2}.$$

The original application of the generalized tree shift was the following theorem. (Unlike the other theorems, this statement has a purely combinatorial proof.)

Theorem 4.11. [2] *Let $W_k(G)$ denote the number of closed walks of length k. Let T be a tree and let T' be obtained from T by a generalized tree shift.*

Then $W_k(T') \geq W_k(T)$ for every $k \geq 1$.

Remark 4.12. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be the eigenvalues of the adjacency matrix of the graph G. Then

$$W_k(G) = \sum_{j=1}^{n} \mu_j^k.$$

Thus the following theorem is an easy consequence of the previous statement.

Corollary 4.13. [2] *Let $EE(G) = \sum_{j=1}^{n} e^{\mu_j}$ denote the Estrada index of the graph G. Let T be a tree and let T' be obtained from T by a generalized tree shift.*

Then $EE(T') \geq EE(T)$.

Remark 4.14. The conjecture concerning the Estrada index prompted V. Nikiforov to state the conjecture that the minimal value of $W_k(G)$ is attained at the path on n vertices among the trees on n vertices. The generalized trees shift was developed to attack this conjecture.

5. Density Turán problem

The following problem was studied in Zoltán L. Nagy's master thesis [8]. This part is based on a joint work with him.

Given a simple, connected graph H. Define the blown-up graph $G[H]$ of H as follows. Replace all vertices $v_i \in V(H)$ by a cluster A_i and we connect vertices between the clusters A_i and A_j (not necessarily all) if v_i and v_j were adjacent in H. Question: what kind of edge densities we have to require between the clusters so that $G[H]$ surely contains a graph isomorph with H such that the vertex corresponding to $v \in V(H)$ is in the cluster corresponding to v. In what follows we call this phenomenon that H is a transversal of $G[H]$.

In the sequel we need some technical definitions.

Definition 5.1. [8, 9] A weighted blown-up graph is a blown-up graph where a non-negative weight $w(u)$ is assigned to each vertex u such that the total weight of each cluster is 1. The density between two clusters is

$$d_{ij} = \sum_{\substack{(u,v)\in E \\ u\in A_i, v\in A_j}} w(u)w(v).$$

Definition 5.2. [8, 9] We define the critical edge density $d_{crit}(H)$ of the graph H as follows. The number $d_{crit}(H)$ is the smallest number d for which it is true that whenever the edge density between any two clusters of $G[H]$ is larger than d then H is surely a transversal of $G[H]$.

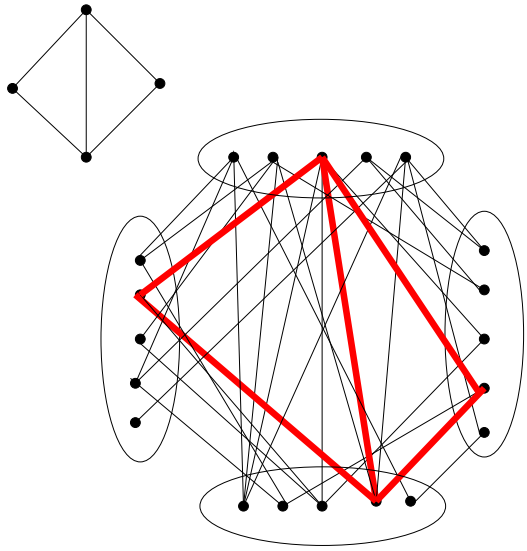

FIGURE 4. A blown-up graph of the diamond containing the diamond as a transversal

Definition 5.3. [6] Let x_e's be variables assigned to each edge of a graph. The *multivariate matching polynomial* F is defined as follows:

$$F(\underline{x_e}, t) = \sum_{M \in \mathcal{M}} (\prod_{e \in M} x_e)(-t)^{|M|},$$

where the summation goes over the matchings of the graph including the empty matching.

Now we are ready to tell out our results. First we study the case when the graph H is a tree.

Theorem 5.4. [6] *Let T be a tree.*

(a) Assume that the edge density between the clusters A_i, A_j of the blown-up graph $G[H]$ is $\gamma_{ij} = 1 - r_{ij}$. Assume that $F_T(\underline{r_e}, t) > 0$ for $t \in [0, 1]$. Then $G[T]$ surely contains T as a transversal.

(b) If for the numbers $\gamma_{ij} = 1 - r_{ij}$, the polynomial $F_T(\underline{r_e}, t)$ has a root in the interval $[0, 1]$ then there exists weighted blown-up graph $G[T]$ of the tree T such that the edge density between the clusters A_i, A_j is γ_{ij}, till $G[T]$ does not contain T as a transversal.

Corollary 5.5. [9] *Let T be a tree and $\mu(T)$ be the largest eigenvalue of the adjacency matrix of T. Then*

$$d_{crit}(T) = 1 - \frac{1}{\mu(T)^2}.$$

If H is an arbitrary graph then the following statements remain true from the above theorems.

Theorem 5.6. [6] *Let H be a simple graph. Assume that the edge density between the clusters A_i, A_j of the blown-up graph $G[H]$ is $\gamma_{ij} = 1 - r_{ij}$. Assume that $F_H(\underline{r_e}, t) > 0$ for $t \in [0, 1]$. Then $G[H]$ surely contains H as a transversal.*

Theorem 5.7. [6] *Let H be a simple graph and let $t(H)$ denote the largest root of the matching polynomial of H. Then*

$$d_{crit}(H) \leq 1 - \frac{1}{t(H)^2}.$$

Corollary 5.8. [6] *Let H be a simple graph with largest degree Δ. Then*

$$1 - \frac{1}{\Delta} \leq d_{krit}(H) < 1 - \frac{1}{4(\Delta - 1)}.$$

As a lower bound we managed to prove the following theorem. Before we give the statement we need some definitions.

Definition 5.9. A *proper labeling* of the vertices of the graph H is a bijective function f from $\{1, 2, \ldots, n\}$ to the set of vertices such that the vertex set $\{f(1), \ldots, f(k)\}$ induces a connected subgraph of H for all $1 \leq k \leq n$. The set of the proper labelings will be denoted by $\mathcal{S}(H)$.

The *monotone-path tree* $T_f(H)$ of H is defined as follows. The vertices of this graph are the paths of the form $f(i_1)f(i_2)\ldots f(i_k)$ where $1 = i_1 < i_2 < \cdots < i_k$ and two such paths are connected if one is the extension of the other with exactly one new vertex.

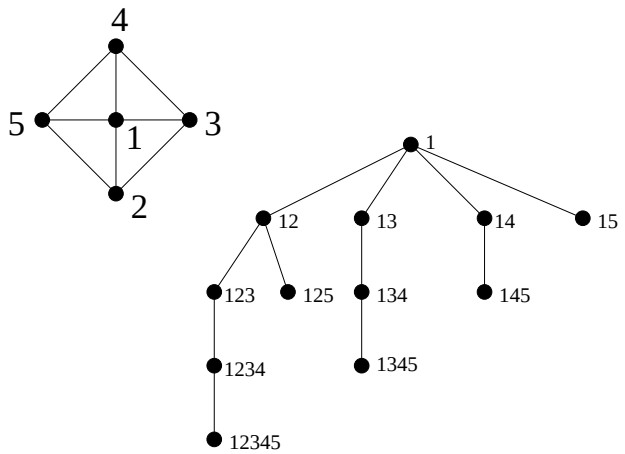

FIGURE 5. A monotone-path tree of the wheel on 5 vertices.

Theorem 5.10. [6]

$$d_{crit}(H) \geq \max_{f \in S(H)} \left\{ 1 - \frac{1}{\mu(T_f(H))^2} \right\}.$$

Remark 5.11. In the case of the complete bipartite graph, for arbitrary proper labeling the largest eigenvalue of the monotone-path tree is $\sqrt{m+n-1}$. So the following conjecture is very natural.

Conjecture 5.12. [6]

$$d_{crit}(K_{n,m}) = 1 - \frac{1}{m+n-1}.$$

6. Integral trees

We call a tree *integral tree* if all the eigenvalues of the tree are integers. The integral trees are extremely rare, among the trees on at most 50 vertices only 28 are integral. Among the 2262366343746 trees on 35 vertices there is only one tree which is integral. In spite of this fact, there were known several infinite class of integral trees, all of them had diameter at most 10. It was an open question for more than 30 years whether there exists integral trees of arbitrarily large diameters. We managed to answer this question affirmatively.

Theorem 6.1. [3] *For every finite set S of positive integers there exists a tree whose positive eigenvalues are exactly the elements of S. If the set S is different from the set $\{1\}$ then the constructed tree will have diameter $2|S|$.*

In the previous section we have seen that the monotone-path tree of the complete bipartite graph $K_{n,m}$ has spectral radius $\sqrt{n+m-1}$. Indeed, the following stronger statement is also true.

Theorem 6.2. *Let f be proper labeling of the complete bipartite graph $K_{n,m}$. Then all the eigenvalues of the monotone-path tree $T_f(K_{n,m})$ have the form $\pm\sqrt{q}$ where q is non-negative integer.*

Hence to prove the above mentioned theorem all we have to prove is that one can put perfect squares under the square roots, this can be done indeed.

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