SPECTRA OF COPIES OF BETHE TREES ATTACHED TO PATH AND APPLICATIONS

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A b s t r a c t. The Bethe tree $B_{d,k}$ is the rooted tree of k levels whose root vertex has degree d, the vertices from level 2 to level k-1 have degree d+1, and the vertices at level k have degree 1. This paper gives a decomposition of the characteristic polynomial of the adjacency matrix of the tree T(d, k, r), obtained by attaching copies of B(d, k) to the vertices of the r-vertex path. Moreover, lower and upper bounds for the energy of T(d, k, r) are obtained.

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1. Introduction

Let G be a simple graph on n vertices. If we label its vertices by $1, \ldots, n$, then its adjacency matrix is given by $A(G) = (a_{i,j})$, where $a_{i,j} = 1$ if the vertex *i* is connected, by an edge of G, to the vertex *j*, and $a_{i,j} = 0$ otherwise. The characteristic polynomial of A(G) is known as the characteristic polynomial of the graph G. The eigenvalues of A(G), same as the zeros of the characteristic polynomial, form the spectrum of G [1]. The eigenvalues of G are denoted by $\lambda_j = \lambda_j(G)$, $j = 1, \ldots, n$, and labelled so that

$$\lambda_1 \leq \cdots \leq \lambda_n$$
 .

The concept of the energy of G, defined as

$$E(G) = \sum_{j=1}^{n} |\lambda_j|$$

was introduced by one of the present authors (see [5, 6] and the references cited therein). Nikiforov [10] defines the energy of a matrix M (square or not) as the sum of its singular values. Recall that if M is a symmetric matrix, then its singular values and the moduli of its eigenvalues coincide.

Let k > 1. A generalized Bethe tree B_k of k levels [13] is a rooted tree in which vertices at same level have the same degree. For $j = 1, \ldots k$, we denote by d_{k-j+1} and by n_{k-j+1} the degree of the vertices at the level j and their number, respectively. Thus, $d_1 = 1$ is the degree of the vertices at the level k (pendent vertices) and d_k is the degree of the root vertex. On the other hand, it is $n_k = 1$, pertaining to the single vertex at the first level, the root vertex. The ordinary Bethe tree $B_{d,k}$ is the rooted trees of k levels whose root vertex has degree d, the vertices from levels 2 to k - 1 have degree d + 1, and the vertices at level k have degree 1.

Spectral properties of Bethe trees (both ordinary and generalized) were much studied in the past. Heilmann and Lieb [7] have determined the decomposition of the matching polynomial of $B_{d,k}$. Recall that the matching and characteristic polynomials of trees coincide [2].

Other spectral properties of Bethe and similar trees were considered in [4, 12, 14, 15]. Eventually, Rojo and one of the present authors found explicit formulas for the eigenvalues of the Bethe trees [16]. With these results the authors in [11] obtained an explicit formula for the energy of the Bethe tree $B_{d,k}$.

Let P_r and C_r be, respectively, the *r*-vertex path and the *r*-vertex cycle. In the paper [13] the spectrum of the graph obtained by attaching copies of $B_{d,k}$ to the vertices of C_r was determined. In this paper we obtain an analogous decomposition of the characteristic polynomial of the tree T(d, k, r), obtained by attaching copies of $B_{d,k}$ to the vertices of P_r . Using this result, lower and upper bounds for the energy of T(d, k, r) are established.

The tree T(2, 4, 3) is depicted in Fig. 1.



Fig. 1. The tree T(2, 4, 3)

In connection with the graphs considered in [13] and in this article, one needs to recall the following result of Godsil and McKay [3].

Denote by $\phi(H, x)$ the characteristic polynomial of a graph H. Let G be a graph on n vertices. Let R be a rooted graph and v its root. Construct the graph product G[R] by attaching a copy of R, via its root, to each vertex of G.

Then $\phi(G[R], x)$, the characteristic polynomial of G[R], is equal to

$$\phi(R-v,x)^n \phi\left(G, \frac{\phi(R,x)}{\phi(R-v,x)}\right) . \tag{1}$$

Evidently, the above formula is applicable to the trees T(d, k, r). Some of the results of the present paper could have been obtained by using the Godsil–McKay formula. Yet, our reasoning follows a somewhat different path.

The present paper has five sections. In this section we recall some results from Matrix Theory. The main result in the second section is

Theorem 1. The characteristic polynomial of the tree T = T(d, k, r) has the following decomposition:

$$\det(\lambda I - A(T)) = \left(\prod_{j \in \Omega} Q_j^{n_j - n_{j+1}}(\lambda)\right)^r \left(\prod_{\ell=1}^r Q_{\ell,k}(\lambda)\right)$$
(2)

where $Q_{\ell,k}(\lambda)$, $\ell = 1, \ldots, r$, is the characteristic polynomial of the matrix $T_{\ell,k}$ in Eq. (12), whereas $Q_j(\lambda)$, $j = 1, \ldots, k-1$, is the characteristic polynomial of the $j \times j$ leading principal submatrix of $T_{\ell,k}$.

In the third section, as an application of Theorem 1, we show that the energy of the tree T(d, 2, r) is equal to

$$4\sum_{\ell=1}^{\lfloor r/2 \rfloor} \sqrt{d + \cos^2 \frac{\ell \pi}{r+1}} \quad \text{if } r \text{ is even} \tag{3}$$

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$$2\sqrt{d} + 4\sum_{\ell=1}^{\lfloor r/2 \rfloor} \sqrt{d + \cos^2 \frac{\ell\pi}{r+1}} \quad \text{if } r \text{ is odd }.$$

$$\tag{4}$$

We denote by E(N) the energy of any matrix N.

Let $M = M(\alpha, h)$ be the $k \times k$ tridiagonal symmetric matrix, specified in Eq. (17). In an earlier work [11] we proved the following

Theorem 2. The energy of $M(\alpha, 0)$ is equal to

$$E(M(\alpha, 0)) = 2\alpha \left(\frac{\sin(\lfloor k/2 \rfloor + 1/2)\frac{\pi}{k+1}}{\sin \frac{\pi}{2(k+1)}} - 1 \right) .$$

In the fourth section we obtain lower and upper bounds for the energy of a $M = M(\alpha, h)$, for $\alpha > 0$, $h \ge 0$.

Let $\alpha, h > 0$. Let $k \ge 3$. Let b := b(k) be defined by

$$b := \frac{\sin(\lfloor k/2 \rfloor + 1/2)\frac{\pi}{k}}{\sin\frac{\pi}{2k}} - 1 .$$
 (5)

We denote by $B(\mu)$ an upper bound for the greatest eigenvalue μ of the matrix $M(\alpha, h)$.

Theorem 3. The energy $E(M(\alpha, h))$ of the matrix $M(\alpha, h)$, defined via Eq. (17), is bounded by

$$-2\alpha\cos\frac{\pi}{k} < E(M(\alpha, h)) - 2\alpha\left(b + \cos\frac{\pi}{k+1}\right) < B(\mu)$$

whenever k is even and

$$-2\alpha\cos\frac{\pi}{k} < E(M(\alpha,h)) - 2\alpha\left(b + \cos\frac{\pi}{k+1}\right) < B(\mu) - 2\alpha\cos\frac{\lfloor k/2\rfloor\pi}{k}$$

whenever k is odd, where b is given by Eq. (5).

Finally, in the last section we search for an upper bound $B(\mu)$. We prove

Theorem 4. Let $\alpha, h > 0$. The greatest eigenvalue μ of the matrix $M(\alpha, h)$, defined via Eq. (17), is bounded by $B(\mu) = \min\{B_1(\mu), B_2(\mu)\}$, where

$$B_1(\mu) = \max\left\{2\alpha \cos\frac{\pi}{2k+1}, \ 2h\cos\frac{\pi}{2k+1}\right\} \ and \ B_2(\mu) = \max\{2\alpha, \ \alpha+h\}.$$

In the fifth section we also obtain lower and upper bounds for the energy of the tree T(d, k, r).

* * * *

We recall that the Kronecker product $A \otimes B$ of a pair of matrices $A = (a_{i,j})$ and $B = (b_{i,j})$ of orders $r \times s$ and $p \times q$, respectively, is the $rp \times sq$ matrix, defined by [9]

$$A \otimes B = \left(\begin{array}{ccc} a_{11}B & \dots & a_{1s}B \\ \vdots & \ddots & \vdots \\ a_{r1}B & \dots & a_{rs}B \end{array}\right) \ .$$

This binary operation has the following properties:

- 1. $(A \otimes B)^T = A^T \otimes B^T$.
- 2. $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$ provided that the matrices A^{-1} and B^{-1} exist.
- 3. $(A \otimes B)(C \otimes D) = (AC \otimes BD)$ provided that the products AC and BD exist.
- 4. $(I_r \otimes I_s) = I_{rs}$, where for a positive integer ℓ , I_ℓ denotes the identity matrix of order ℓ .
- 5. $(I_r \otimes B) = diag(B, \ldots, B)$.

We denote by $\lambda_p(N)$ the p-th eigenvalue of any matrix N and we recall the following Lemmas.

Lemma 5 (Monotonicity Theorem) [8]. Let A, B be $k \times k$ real and symmetric matrices. Let

$$C = A + B$$

and let $\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_k(A)$, $\lambda_1(B) \leq \lambda_2(B) \leq \cdots \leq \lambda_k(B)$, and $\lambda_1(C) \leq \lambda_2(C) \leq \cdots \leq \lambda_k(C)$ be the ordered eigenvalues of A, B, and C, respectively. Then

$$\lambda_j(A) + \lambda_{i-j+1}(B) \le \lambda_i(C)$$

whenever $i \geq j$ and

$$\lambda_i(C) \leq \lambda_j(A) + \lambda_{i-j+k}(B)$$

whenever $i \leq j$.

Lemma 6. (Interlacing Cauchy Theorem) [8]. Let

$$A = \left[\begin{array}{cc} B & C \\ C^T & D \end{array} \right]$$

be a $k \times k$ symmetric matrix, where B is a $j \times j$ principal submatrix of A. Let $\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_k(A)$, $\lambda_1(B) \leq \cdots \leq \lambda_j(B)$ be the ordered eigenvalues of A and B respectively. Then for $\ell = 1, \ldots j$,

$$\lambda_{\ell}(A) \leq \lambda_{\ell}(B) \leq \lambda_{\ell+k-j}(A)$$
.

Lemma 7. Let A be an $m \times m$ symmetric tridiagonal matrix with nonzero codiagonal entries. Then the eigenvalues of any $(m-1) \times (m-1)$ principal submatrix strictly interlace the eigenvalues of A.

The following result is known as the three-term recursion formula for tridiagonal symmetric matrices. The characteristic polynomials, $\tilde{Q}_j(\lambda)$, of the $j \times j$ leading principal submatrices of the symmetric tridiagonal matrix

$$A_{k} = \begin{bmatrix} a_{1} & b_{1} & & \\ b_{1} & \ddots & \ddots & \\ & \ddots & \ddots & b_{k-1} \\ & & b_{k-1} & a_{k} \end{bmatrix}$$

satisfy the following three-term recursion formula

$$\widetilde{Q}_{j}(\lambda) = (\lambda - a_{j})\widetilde{Q}_{j-1}(\lambda) - b_{j-1}^{2}\widetilde{Q}_{j-2}(\lambda) , \ j = 2, \dots, k$$
(6)

where

$$\tilde{Q}_0(\lambda) = 1$$
 and $\tilde{Q}_1(\lambda) = \lambda - a_1$.

Let L > 0. In [11] it was shown that

$$\sum_{k=1}^{n} \left(2\cos\frac{k\pi}{L} \right) = \frac{\sin(n+1/2)\frac{\pi}{L}}{\sin\frac{\pi}{2L}} - 1 .$$
 (7)

2. Characteristic polynomial of T(d, k, r)

We observe that on the level j, j = 1, ..., k of the tree T := T(d, k, r), there are $r n_{k-j+1}$ vertices. Hence and if n denotes the order of adjacency matrix, we see that $n = r \sum_{j=1}^{k} n_j$.

From our notation for the tree B_k it is clear that

$$n_{k-j} = (d_{k-j+1} - 1)n_{k-j+1}$$
, $j = 1, \dots, k-1$ and $n_{k-1} = d_k$

Here and in what follows **0** denotes the all-zero matrix; its order is clear from the context. For a positive integer ℓ let $\mathbf{e}_{\ell} = (\mathbf{1}, \ldots, \mathbf{1})^{\mathbf{T}}$, the all-one vector of order ℓ . Let

$$m_j = \frac{n_j}{n_{j+1}}$$
, $j = 1, \dots, k-1$.

Hence,

$$m_i = d_{i+1} - 1$$
, $j = 1, \ldots, k - 2$

and

$$m_{k-1} = d_k \; .$$

Let B_j be the block diagonal matrix defined by

$$B_j = I_{n_{i+1}} \otimes \mathbf{e}_{\mathbf{m}_i}$$

with n_{j+1} diagonal blocks equal to $\mathbf{e}_{\mathbf{m}_j}$. We observe that B_j has order $n_j \times n_{j+1}$ and that $B_{k-1} = \mathbf{e}_{\mathbf{n}_{k-1}}$. For $j = 1, \ldots, k-1$, let C_j be the $(r n_j) \times (r n_{j+1})$ block diagonal matrix,

$$C_j = I_r \otimes B_j$$

with r diagonal blocks equal to B_j . Hence C_{k-1} is the $r n_{k-1} \times r$ block diagonal matrix $C_{k-1} = I_r \otimes \mathbf{e_{n_{k-1}}}$, with r diagonal blocks equal to $\mathbf{e_{n_{k-1}}}$.

Consider the tridiagonal symmetric $r \times r$ matrices

$$F_r = \begin{bmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{bmatrix}$$
(8)

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and

$$M_r = \alpha F_r . \tag{9}$$

Observe that F_r is the adjacency matrix of the path P_r . It is well known that [1]

$$\lambda_{\ell}(M_r) = 2\alpha \cos \frac{(r+1-\ell)\pi}{r+1} , \ \ell = 1, \dots, r$$

Therefore, $\lambda_{\ell}(M_r) = -\lambda_{r+1-\ell}(M_r)$, $\ell = 1, \ldots, r$. Moreover if r is odd, then $\lambda_{(r+1)/2}(M_r) = 0$.

In view of our labelling, the adjacency matrix of T(d, k, r) becomes equal to the following block tridiagonal matrix:

$$A(T(d,k,r)) = \begin{bmatrix} 0 & C_1 & & \\ C_1^T & \ddots & \ddots & \\ & \ddots & 0 & C_{k-1} \\ & & C_{k-1}^T & F_r \end{bmatrix}$$

Lemma 8. For j = 1, ..., k, let $\alpha_j := \alpha_j(\lambda)$ be a polynomial with real coefficients, and

$$M_{1} = \begin{bmatrix} \alpha_{1} I_{r n_{1}} & -C_{1} & & \\ -C_{1}^{T} & \ddots & \ddots & \\ & \ddots & \alpha_{k-1} I_{r n_{k-1}} & -C_{k-1} \\ & & -C_{k-1}^{T} & \alpha_{k} I_{r} - F_{r} \end{bmatrix}$$

Moreover let

$$\beta_1 = \alpha_1$$

and $\beta_{j-1}(\lambda) \neq 0$,

$$\beta_j = \alpha_j - \frac{n_{j-1}}{n_j} \frac{1}{\beta_{j-1}}$$

for j = 2, 3, ..., k. Then for all real λ , such that $\beta_j(\lambda) \neq 0$, j = 1, 2, ..., k - 1,

$$\det M_1 = \left(\beta_1^{n_1}\beta_2^{n_2}\cdots\beta_{k-1}^{n_{k-1}}\right)^r \prod_{\ell=1}^r \left(\beta_k - 2\cos\frac{\ell\pi}{r+1}\right) .$$
(10)

Proof. For the matrix M_1 we proceed as in Gaussian elimination, but this time we use the blocks. Thus for j = 1, ..., k-1 and $\beta_j \neq 0$, the matrix C_j^T is eliminated with $\beta_j I_{rn_j}$, in consequence $\alpha_{j+1} I_{rn_{j+1}}$ is replaced by $\alpha_{j+1} I_{rn_{j+1}} - \beta_j^{-1} C_j^T C_j I_{rn_j}$. Via definition of matrices B_j and C_j and the above properties of Kronecker product, we prove directly that $C_j^T C_j I_{rn_j} = m_j I_{rn_{j+1}} = \frac{n_j}{n_{j+1}} I_{rn_{j+1}}$. Then

$$\alpha_{j+1} I_{r n_{j+1}} - \beta_j^{-1} C_j^T C_j I_{r n_j} = \beta_{j+1} I_{r n_{j+1}} .$$

Finally this process yields the matrix

$$\alpha_k I_r - F_r - n_{k-1} I_r = \beta_k I_r - F_r$$

By a similar reasoning as in the Gaussian elimination, it is possible to show that the determinants of the obtained block upper triangular matrix and of M_1 coincide. Eq. (10) follows.

Let $\Omega = \{j = 1, \dots, k - 1 : n_j > n_{j+1}\}$. Consider the polynomials $Q_0(\lambda) = 1, Q_1(\lambda) = \lambda$ and

$$Q_j(\lambda) = \lambda Q_{j-1}(\lambda) - \frac{n_{j-1}}{n_j} Q_{j-2}(\lambda) , \ j = 2, \dots, k-1 .$$

Finally let

$$Q_{\ell,k}(\lambda) = \left(\lambda - 2\cos\frac{\ell\pi}{r+1}\right)Q_{k-1}(\lambda) - \frac{n_{k-1}}{n_k}Q_{k-2}(\lambda) , \ \ell = 1, \dots, r .$$

Theorem 1 can now be derived from Lemma 8.

P r o o f of Theorem 1. We apply Lemma 8 to the matrix $M_1 = \lambda I - A(T)$. For this matrix,

$$\alpha_j = \lambda$$
, $j = 1, \ldots, k$.

Suppose that $\lambda \in \mathbb{R}$ is such that $Q_j(\lambda) \neq 0$ for all $j = 1, \ldots, k-1$. We have

$$\begin{split} \beta_1 &= \lambda = \frac{Q_1}{Q_0} \neq 0, \\ \beta_2 &= \lambda - \frac{1}{\beta_1} \frac{n_1}{n_2} = \frac{\lambda Q_1 - \frac{n_1}{n_2} Q_0}{Q_1} = \frac{Q_2}{Q_1} \neq 0, \end{split}$$

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$$\beta_{k-1} = \lambda - \frac{1}{\beta_{k-2}} \frac{n_{k-2}}{n_{k-1}} = \frac{Q_{k-1}}{Q_{k-2}} \neq 0$$

$$\beta_k - 2\cos\frac{\pi\ell}{r+1} = \lambda - 2\cos\frac{\pi\ell}{r+1} - \frac{n_{k-1}}{n_k}\frac{1}{\beta_{k-1}}$$

$$= \left(\lambda - 2\cos\frac{\pi\ell}{r+1}\right) - \frac{n_{k-1}}{n_k}\frac{Q_{k-2}}{Q_{k-1}} = \frac{Q_{\ell,k}}{Q_{k-1}} .$$

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From Eq. (10) we obtain

$$\det(\lambda I - A(T)) = \left(\prod_{j=1}^{k-1} \beta_j^{n_j}\right)^r \prod_{\ell=1}^r \left(\beta_k - 2\cos\frac{\pi\ell}{r+1}\right) = \left(\prod_{j\in\Omega} Q_j^{n_j - n_{j+1}}\right)^r \prod_{\ell=1}^r Q_{\ell,k} .$$
(11)

Thus, (2) is proved for all $\lambda \in \mathbb{R}$, such that $Q_j(\lambda) \neq 0$, $j = 1, \ldots, k - 1$.

Suppose now that $Q_j(\lambda_0) = 0$ for some j and for some $\lambda_0 \in \mathbb{R}$. Since the zeros of any nonzero polynomial are isolated, there exists a neighborhood $N(\lambda_0)$ of λ_0 such that $Q_{\ell}(\lambda) \neq 0$ for all $\lambda \in N(\lambda_0) \setminus \{\lambda_0\}$ and for all $\ell = 1, \ldots, k - 1$. Hence (11) is proved for all $\lambda \in N(\lambda_0) \setminus \{\lambda_0\}$. By continuity, taking the limit as $\lambda \to \lambda_0\,,$ we have

$$\det(\lambda_0 I - A(T)) = \left(\prod_{j \in \Omega} Q_j^{n_j - n_{j+1}}(\lambda_0)\right)^r \prod_{\ell=1}^r Q_{\ell,k}(\lambda_0) \ .$$

Therefore (2) holds for all $\lambda \in \mathbb{R}$.

For $\ell = 1, \ldots, r$, let $T_{\ell,k}$ be the following $k \times k$ symmetric tridiagonal matrix

$$\begin{bmatrix} 0 & \sqrt{d_2 - 1} & & & \\ \sqrt{d_2 - 1} & 0 & \ddots & & \\ & \ddots & \ddots & \sqrt{d_{k-1} - 1} & \\ & & \sqrt{d_{k-1} - 1} & 0 & \sqrt{d_k} \\ & & & \sqrt{d_k} & 2\cos\frac{\ell\pi}{r+1} \end{bmatrix}.$$
 (12)

For j = 1, ..., k - 1, let T_j be the $j \times j$ leading principal submatrix of $T_{1,k}$. The following result is a direct consequence of relation (6).

Lemma 9. For
$$j = 1, 2, ..., k - 1$$
,
 $det(\lambda I - T_j) = Q_j(\lambda)$ (13)

and for $\ell = 1, 2, ..., r$,

$$\det(\lambda I - T_{\ell,k}) = Q_{\ell,k}(\lambda) .$$
(14)

In particular, when we attach r copies of the tree $B_{d,k}$ to the vertices of P_r , then the matrices in (12) (pertaining to A(T(d,k,r))) become the following irreducible matrices, [8]:

$$S(\ell, k, r) = \begin{bmatrix} 0 & \sqrt{d} & & \\ \sqrt{d} & \ddots & \ddots & \\ & & & \\ & \ddots & 0 & \sqrt{d} \\ & & \sqrt{d} & 2\cos\frac{\ell\pi}{r+1} \end{bmatrix}, \ \ell = 1, \dots, r \ . \tag{15}$$

Moreover for j = 1, ..., k-1, the submatrices T_j , are equal to the matrices $S_j = \sqrt{d} F_j$ where the matrix F_j is as in (8). The energy of these matrices is given by [11]

$$E(S_j) = 2\sqrt{d} \left(\frac{\sin(\lfloor j/2 \rfloor + 1/2)\frac{\pi}{j+1}}{\sin\frac{\pi}{2(j+1)}} - 1 \right) , \ j = 1, \dots, k-1 .$$

Moreover [7],

$$n_j - n_{j+1} = d^{k-1-j} \left(d - 1 \right) \,. \tag{16}$$

We denote by S_k the matrix $\sqrt{d} F_k$, where F_k is as in (8). For matrices in (15) we observe,

$$\lambda_p(S(\ell, k, r)) = -\lambda_{k+1-p}(S(r+1-\ell, k, r)) , \ p = 1, \dots, k \ , \ \ell = 1, \dots, r \ .$$

For $r \geq 2$ this property and the definition of energy imply

$$E(S(\ell, k, r)) = E(S(r + 1 - \ell, k, r)), \ \ell = 1, \dots, \lfloor r/2 \rfloor.$$

For odd r and $\ell = 1 + \lfloor r/2 \rfloor$, it is $2 \cos \frac{\ell \pi}{r+1} = 0$, which implies $S(1 + \lfloor r/2 \rfloor, k, r) = S_k$. Therefore we obtain [11],

$$E(S(1+\lfloor r/2\rfloor,k,r)) = 2\sqrt{d} \left(\frac{\sin(\lfloor k/2\rfloor+1/2)\frac{\pi}{k+1}}{\sin\frac{\pi}{2(k+1)}} - 1\right) .$$

The following Lemma is a consequence of Theorem 1 and Lemmas 5, 6 and 7.

Lemma 10. Let
$$1 \leq \ell_1 \leq \ell_2 \leq \lfloor r/2 \rfloor$$
. Then,
a) $\lambda_p(S(\ell_2, k, r)) \leq \lambda_p(S(\ell_1, k, r))$, $p = 1, \dots, k$,
b) $\lambda_p(S(\ell, k, r)) < \lambda_p(S_j) < \lambda_{p+k-j}(S(\ell, k, r))$, $p = 1, \dots, j$, $\ell = 1, \dots, \lfloor r/2 \rfloor$.

c) The greatest $\lfloor r/2 \rfloor$ eigenvalues of the tree T(d, k, r) are the greatest eigenvalues of the matrices $S(\ell, k, r)$, $\ell = 1, \ldots, \lfloor r/2 \rfloor$, whenever r is an even number, and the greatest $\lfloor r/2 \rfloor + 1$ eigenvalues of the tree T(d, k, r) are the greatest $\lfloor r/2 \rfloor + 1$ eigenvalues of $S(\ell, k, r)$, $\ell = 1, \ldots, \lfloor r/2 \rfloor + 1$, whenever r is an odd number.

d) The greatest eigenvalue of T(d, k, r) is $\lambda_k(S(1, k, r))$.

Proof. Note that $S(\ell_1, k, r) = S(\ell_2, k, r) + B$, where $B = \begin{bmatrix} \mathbf{0} & 0 \\ 0^T & g \end{bmatrix}$, g > 0. By Lemma 5 we have

$$\lambda_q(S(\ell_2,k,r)) + \lambda_{p-q+1}(B) \leq \lambda_p(S(\ell_1,k,r)) \ , \ p \geq q$$

We obtain the first result by taking q = p. The second result is obtained by observing that S_j is a $j \times j$ submatrix of the matrix $S(\ell, k, r)$ and by applying Lemma 6. The facts c) and d) are obtained as consequence of the Theorem 1 and of a) and b).

3. Example: The energy of T(d, 2, r)

In this section, in order to exemplify the general theory from the previous section, we compute the spectrum and energy of T(d, 2, r). The same results could have been obtained also by using the Godsil–McKay formula (1). The figure below corresponds to T(2, 2, 8).



Fig. 2. The tree T(2, 2, 8).

For the tree T(d, 2, r) the matrices in (15) reduce to the following 2×2 matrices:

$$S(\ell, 2, r) = \begin{bmatrix} 0 & \sqrt{d} \\ \sqrt{d} & 2\cos\frac{\ell\pi}{r+1} \end{bmatrix}, \ \ell = 1, \dots, \lfloor r/2 \rfloor$$

with eigenvalues

$$\cos\frac{\ell\pi}{r+1} \pm \sqrt{d+\cos^2\frac{\ell\pi}{r+1}} \quad , \quad \ell = 1, \dots, \lfloor r/2 \rfloor \; .$$

All other eigenvalues of T(d, 2, r) are equal to zero. Thus

$$E(S(\ell, 2, r)) = \left| \cos \frac{\ell \pi}{r+1} + \sqrt{d + \cos^2 \frac{\ell \pi}{r+1}} \right| + \left| \cos \frac{\ell \pi}{r+1} - \sqrt{d + \cos^2 \frac{\ell \pi}{r+1}} \right|$$
$$= 2\sqrt{d + \cos^2 \frac{\ell \pi}{r+1}}.$$

Then the decomposition in (2) and the matrices in (15) imply

Theorem 11. The energy E(T(d, 2, r)) is given by Eqs. (3) and (4).

4. Bounds for the energy of certain matrices

Let $\alpha > 0$ and $h \ge 0$. Consider the tridiagonal symmetric $k \times k$ matrix

$$M := M(\alpha, h) = \begin{bmatrix} M_{k-1} & (0, 0, \dots, 0, \alpha)^T \\ (0, 0, \dots, 0, \alpha) & h \end{bmatrix}$$
(17)

where $M_{k-1} = \alpha F_{k-1}$ is given by Eq. (9). Then,

$$\lambda_j(M_{k-1}) = 2\alpha \cos \frac{(k-j)\pi}{k} , \ j = 1, \dots, k-1 .$$
 (18)

Lemma 12a. Let k = 2p. Then for i = 2, ..., k - 1,

$$2\alpha \cos \frac{i\pi}{k} < |\lambda_i(M)| < 2\alpha \cos \frac{(i-1)\pi}{k} , \ i = 2, \dots, p$$
(19)

and

$$2\alpha \cos \frac{(k-i+1)\pi}{k} < |\lambda_i(M)| < 2\alpha \cos \frac{(k-i)\pi}{k} , \ i = p+1, \dots, k-1 .$$
 (20)

P r o o f. We consider the ordered eigenvalues

$$\lambda_1(M) \leq \lambda_2(M) \leq \cdots \leq \lambda_k(M)$$
.

By Lemmas 5 and 6, and by using the eigenvalues in (18), we derive,

$$2\alpha \cos \frac{(k-i+1)\pi}{k} < \lambda_i(M) < 2\alpha \cos \frac{(k-i)\pi}{k} , \ i = 2, \dots, k-1 .$$
 (21)

Hence, if $i \leq p$ then $2\alpha \cos \frac{(k-i)\pi}{k} \leq 0$ implying $\lambda_i(M) < 0$. By multiplying in (21) by (-1) the inequalities in (19) are obtained. In a same way, if $i \geq p+1$, then by $2\alpha \cos \frac{(k-i+1)\pi}{k} > 0$ we have $\lambda_i(M) \geq 0$, and (20) follows from (21).

Lemma 12b. Let k = 2p + 1. Then

$$2\alpha \cos \frac{i\pi}{k} < |\lambda_i(M)| < 2\alpha \cos \frac{(i-1)\pi}{k} , \ i = 2, \dots, p$$
(22)

$$0 \le |\lambda_{p+1}(M)| < 2\alpha \cos \frac{p\pi}{k} \tag{23}$$

and

$$2\alpha \cos \frac{(k-i+1)\pi}{k} < |\lambda_i(M)| < 2\alpha \cos \frac{(k-i)\pi}{k} , \ i = p+2, \dots, k-1 .$$
 (24)

P r o o f. As before, the inequalities (21) imply (22). For i = p + 1 in (21) we obtain

$$2\alpha \cos \frac{(p+1)\pi}{2p+1} < \lambda_{p+1}(M) < 2\alpha \cos \frac{p\pi}{2p+1}$$
.

Hence, by using the identity

$$\cos\frac{(p+1)\pi}{2p+1} = -\cos\frac{p\pi}{2p+1}$$

we arrive at (23). If $i \ge p+2$, then $2\alpha \cos \frac{(k-i+1)\pi}{k} > 0$. Therefore, (24) follows directly from (21).

Let b := b(k) be defined as

$$b := \sum_{i=1}^{\lfloor k/2 \rfloor} \left(2\cos\frac{i\pi}{k} \right) = \frac{\sin(\lfloor k/2 \rfloor + 1/2)\frac{\pi}{k}}{\sin\frac{\pi}{2k}} - 1 \tag{25}$$

where the last identity is implied by (7).

Lemma 13. Let k be an even number. Let b be as in (25). Consider the tridiagonal symmetric $k \times k$ matrix $M = M(\alpha, h)$, Eq. (17), and suppose that $a_1 < |\lambda_1(M)| < b_1$ and $a_k < |\lambda_k(M)| < b_k$. Then

$$a_1 + a_k - 4\alpha \cos \frac{\pi}{k} < E(M) - 2\alpha b < b_1 + b_k$$
.

P r o o f. Let k = 2p. Thus $\lfloor k/2 \rfloor = p$. Clearly

$$E(M) = |\lambda_1(M)| + |\lambda_k(M)| + \sum_{i=2}^p |\lambda_i(M)| + \sum_{i=p+1}^{k-1} |\lambda_i(M)| .$$
 (26)

By summation from i = 2 to i = p in the inequalities in (19) we obtain

$$\alpha \sum_{i=2}^{p} 2\cos\frac{i\pi}{k} < \sum_{i=2}^{p} |\lambda_i(M)| < \alpha \sum_{i=2}^{p} 2\cos\frac{(i-1)\pi}{k} .$$

For this case

$$\sum_{i=2}^{p} 2\cos\frac{(i-1)\pi}{k} = \sum_{i=1}^{p} 2\cos\frac{i\pi}{k} = b \; .$$

Thus from the above inequalities and (25) we have

$$\alpha \left(b - 2\cos\frac{\pi}{k} \right) < \sum_{i=2}^{p} |\lambda_i(M)| < \alpha b .$$
(27)

In (20) we take the sum from i = p + 1, to i = k - 1, thus obtaining

$$\alpha \sum_{i=p+1}^{k-1} 2\cos\frac{(k-i+1)\pi}{k} < \sum_{i=p+1}^{k-1} |\lambda_i(M)| < \alpha \sum_{i=p+1}^{k-1} 2\cos\frac{(k-i)\pi}{k} .$$
(28)

By a change of variable,

$$\alpha \sum_{i=p+1}^{k-1} 2\cos\frac{(k-i+1)\pi}{k} = \alpha \sum_{j=2}^{p} 2\cos\frac{j\pi}{k} = \alpha \left(b - 2\cos\frac{\pi}{k}\right)$$

and

$$\alpha \sum_{i=p+1}^{k-1} 2\cos\frac{(k-i)\pi}{k} = \alpha \sum_{j=1}^{p-1} 2\cos\frac{j\pi}{k} = \alpha b$$

Thus, inequalities in (28) and (25) imply

$$\alpha \left(b - 2\cos\frac{\pi}{k} \right) < \sum_{i=p+1}^{k-1} |\lambda_i(M)| < \alpha b .$$
⁽²⁹⁾

Now the result is obtained directly from (26), bounds in (27) and (29) and the bounds given for $|\lambda_1(M)|$ and $|\lambda_k(M)|$.

Lemma 14. Let k be an odd integer. Let b be as in (25) and $M = M(\alpha, h)$ as in (17). Suppose that $a_1 < |\lambda_1(M)| < b_1$ and $a_k < |\lambda_k(M)| < b_k$. Then

$$a_1 + a_k - 4\alpha \cos \frac{\pi}{k} < E(M) - 2\alpha b < b_1 + b_k - 2\alpha \cos \frac{\lfloor k/2 \rfloor \pi}{k}$$
.

P r o o f. Let k = 2p + 1. Thus $\lfloor k/2 \rfloor = p$. Evidently,

$$E(M) = |\lambda_1(M)| + |\lambda_k(M)| + \sum_{i=2}^p |\lambda_i(M)| + \sum_{i=p+2}^{k-1} |\lambda_i(M)| + |\lambda_{p+1}(M)| .$$
(30)

By summation from i = 2 to i = p in (22) we obtain

$$\alpha \sum_{i=2}^{p} 2\cos\frac{i\pi}{k} < \sum_{i=2}^{p} |\lambda_i(M)| < \alpha \sum_{i=2}^{p} 2\cos\frac{(i-1)\pi}{k} .$$

Hence by (25) we directly obtain,

$$\alpha \left(b - 2\cos\frac{\pi}{k} \right) < \sum_{i=2}^{p} |\lambda_i(M)| < \alpha \left(b - 2\cos\frac{p\pi}{k} \right) .$$
(31)

By summing from i = p + 2 to i = k - 1 in (24) we have

$$\alpha \sum_{i=p+2}^{k-1} 2\cos\frac{(k-i+1)\pi}{k} < \sum_{i=p+2}^{k-1} |\lambda_i(M)| < \alpha \sum_{i=p+2}^{k-1} 2\cos\frac{(k-i)\pi}{k} .$$
(32)

By a change of variable,

$$\alpha \sum_{i=p+2}^{k-1} 2\cos\frac{(k-i+1)\pi}{k} = \alpha \sum_{j=2}^{p} 2\cos\frac{j\pi}{k} = \alpha \left(b - 2\cos\frac{\pi}{k}\right)$$

and

$$\alpha \sum_{i=p+2}^{k-1} 2\cos\frac{(k-i)\pi}{k} = \alpha \sum_{j=1}^{p-1} 2\cos\frac{j\pi}{k} = \alpha \left(b - 2\cos\frac{p\pi}{k}\right) .$$

Thus from the inequalities in (32) and by (25) we get

$$\alpha \left(b - 2\cos\frac{\pi}{k} \right) < \sum_{i=p+2}^{k-1} |\lambda_i(M)| < \alpha b - 2\alpha \cos\frac{p\pi}{k} .$$
(33)

The result is directly obtained from (30), bounds in (31), (33), and (23) as well as the bounds given for $|\lambda_1(M)|$ and $|\lambda_k(M)|$.

We recall that for the extreme eigenvalues of the matrix $M(\alpha, 0)$ in (17),

$$|\lambda_1(M(\alpha,0))| = |\lambda_k(M(\alpha,0))| = 2\alpha \cos \frac{\pi}{k+1} .$$

Lemma 15. Let h > 0. Then

$$2\alpha \cos \frac{\pi}{k} < |\lambda_1(M(\alpha, h))| < 2\alpha \cos \frac{\pi}{k+1}$$
(34)

and

$$2\alpha \cos \frac{\pi}{k+1} \le |\lambda_k(M(\alpha, h))| .$$
(35)

P r o o f. Consider the ordered eigenvalues of $M(\alpha, h)$,

$$\lambda_1(M(\alpha, h)) \le \lambda_2 M(\alpha, h)) \le \dots \le \lambda_k(M(\alpha, h))$$

and observe that

$$M(\alpha, h) = \alpha F_k + B$$
 where $B = \begin{bmatrix} \mathbf{0} & 0 \\ 0^T & h \end{bmatrix}$.

By Lemma 5 we have

$$\lambda_j(\alpha F_k) + \lambda_{i-j+1}(B) \le \lambda_i(M(\alpha, h)) , \ i \ge j .$$
(36)

In (36), i = j = 1 imply

$$2\alpha \cos \frac{k\pi}{k+1} + \lambda_1(B) \le \lambda_1(M(\alpha, h)) \; .$$

In this case $\lambda_1(B) = 0$. Therefore

$$2\alpha\cos\frac{k\pi}{k+1} \leq \lambda_1(M(\alpha,h)) \ .$$

On the other hand, by using Lemma 7 we have

$$\lambda_1(M(\alpha, h)) < \lambda_1(M_{k-1}) = 2\alpha \cos \frac{(k-1)\pi}{k} .$$

Therefore

$$2\alpha\cos\frac{k\pi}{k+1} \le \lambda_1(M(\alpha,h)) < 2\alpha\cos\frac{(k-1)\pi}{k}$$

and (34) is obtained by multiplying the above inequalities by (-1). In (36) we consider i = j = k and obtain

$$\lambda_k(M(\alpha, h)) \ge \lambda_k(\alpha F_k) + \lambda_1(B) = 2\alpha \cos \frac{\pi}{k+1}$$

which leads to (35).

Theorem 3 is now obtained as an immediate corollary of Lemmas 13, 14, and 15.

5. Estimating the energy of T(d, k, r)

Proof of Theorem 4. Let

$$P = \begin{bmatrix} F_{k-1} & (0, 0, \dots, 0, 1)^T \\ (0, 0, \dots, 0, 1) & 1 \end{bmatrix}$$

with F_{k-1} given in Eq. (8). Let $v = \max\{\alpha, h\}$. Then $M(\alpha, h) \leq vP$. Both $M(\alpha, h)$ and vP are irreducible matrices. Then by comparing their spectral radii [9] we have

$$\lambda_k(M(\alpha,h)) \le \lambda_k(vP) = 2v \cos \frac{\pi}{2k+1}$$
.

Thus $B_1(\mu)$ is an upper bound of μ . By the Gershgorin theorem [9], $B_2(\mu)$ is an other upper bound of μ . Theorem 4 follows.

Example. For the 20×20 matrix $M(\sqrt{2}, 2)$ defined by taking k = 20 in (17) we have $E(M(\sqrt{2}, 2)) = 35.9051$. Our lower and upper bounds are 31.4536 and 37.6614, respectively.

By applying Theorem 1 to the tree T(d, k, r), the matrices in (15) are obtained. By means of the decomposition (2), and the relations (13), (14), (16), we obtain

$$E(T(d,k,r)) = r \sum_{j=1}^{k-1} d^{k-1-j} (d-1)E(S_j) + 2 \sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r))$$

for r even, and

$$E(T(d, k, r)) = r \sum_{j=1}^{k-1} d^{k-1-j} (d-1)E(S_j) + \sum_{\ell=1}^{\lfloor r/2 \rfloor} 2E(S(\ell, k, r)) + E(S(1 + \lfloor r/2 \rfloor, k, r))$$

for odd r. We recall that $E(B_{d,k})$ denotes the energy of the Bethe tree $B_{d,k}$. In [11] it was proven that

$$\sum_{j=1}^{k-1} d^{k-1-j} \left(d-1 \right) E(S_j) = E(B_{d,k}) - E(S_k) \; .$$

Therefore

$$E(T(d,k,r)) - r E(B_{d,k}) + r E(S_k) = 2 \sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r))$$
(37)

for even r and

$$E(T(d,k,r)) - r E(B_{d,k}) + (r-1)E(S_k) = 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r))$$
(38)

whenever r is odd. For the matrices $M(\alpha, h)$ in (17) and $S(\ell, k, r)$ we obtain

$$S(\ell, k, r) = M\left(\sqrt{d}, 2\cos\frac{\ell\pi}{r+1}\right) , \ \ell = 1, \dots, \lfloor r/2 \rfloor$$

and by the results from Section 4, their energies are bounded as follows, for $\ell = 1, \ldots, \lfloor r/2 \rfloor$,

$$-2\sqrt{d}\cos\frac{\pi}{k} < E(S(\ell,k,r)) - 2\sqrt{d}\left(b + \cos\frac{\pi}{k+1}\right) < B(\ell,k,r)$$

for $\ell = 1, \dots, \lfloor r/2 \rfloor$, and even k, and

$$-2\sqrt{d}\cos\frac{\pi}{k} < E(S(\ell,k,r)) - 2\sqrt{d}\left(b + \cos\frac{\pi}{k+1}\right) < B(\ell,k,r) - 2\sqrt{d}\cos\frac{\lfloor k/2 \rfloor \pi}{k}$$

for $\ell=1,\ldots,\lfloor r/2\rfloor\,,$ and odd $k\,,$ By Theorem 4 we have

$$B(\ell, k, r) = \min\{B_1(\ell, k, r), B_2(\ell, k, r)\}, \ \ell = 1, \dots, \lfloor r/2 \rfloor$$

where

$$B_1(\ell, k, r) = \max\left\{2\sqrt{d}\cos\frac{\pi}{2k+1} , \ 4\cos\frac{\ell\pi}{r+1}\cos\frac{\pi}{2k+1}\right\} , \ \ell = 1, \dots, \lfloor r/2 \rfloor$$

and

$$B_2(\ell, k, r) = \max\left\{2\sqrt{d} , \sqrt{d} + 2\cos\frac{\ell\pi}{r+1}\right\}, \ \ell = 1, \dots, \lfloor r/2 \rfloor.$$

From this we obtain

$$2\sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r)) < 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(b + \cos\frac{\pi}{k+1} \right) + 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$
(39)

and

$$4\left\lfloor \frac{r}{2} \right\rfloor \sqrt{d} \left(b + \cos \frac{\pi}{k+1} - \cos \frac{\pi}{k} \right) < 2 \sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r))$$
(40)

for even k, and

$$2\sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r)) < 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(b + \cos\frac{\pi}{k+1} - \cos\frac{\lfloor k/2 \rfloor \pi}{k} \right) + 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$

$$\tag{41}$$

and

$$4\left\lfloor \frac{r}{2} \right\rfloor \sqrt{d} \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\pi}{k} \right) < 2 \sum_{\ell=1}^{\lfloor r/2 \rfloor} E(S(\ell,k,r)) .$$
 (42)

for odd k.

Then for the energy E(T(d, k, r)), from (37), (39), and (40) we obtain

$$E(T(d,k,r)) - rE(B_{d,k}) + rE(S_k) < 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b \right) + 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$

and

$$4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\pi}{k} \right) < E(T(d,k,r)) - rE(B_{d,k}) + rE(S_k)$$

whenever k and r are even numbers. Moreover from (37), (41), and (42) we obtain

$$E(T(d,k,r)) - rE(B_{d,k}) + rE(S_k)$$

$$< 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\lfloor k/2 \rfloor \pi}{k} \right) + 2 \sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$

and

$$4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\pi}{k} \right) < E(T(d,k,r)) - rE(B_{d,k}) + rE(S_k)$$

whenever r is an even number and k is an odd number.

From (38), (39), and (40) we obtain,

$$E(T(d,k,r)) - rE(B_{d,k}) + (r-1)E(S_k) < 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b \right) + 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$

and

$$4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\pi}{k} \right) < E(T(d,k,r)) - rE(B_{d,k}) + (r-1)E(S_k)$$

whenever r is odd and k is even.

From (38), (41), and (42) we obtain,

$$E(T(d,k,r)) - rE(B_{d,k}) + (r-1)E(S_k)$$

$$< 4\sqrt{d} \left\lfloor \frac{r}{2} \right\rfloor \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\lfloor k/2 \rfloor \pi}{k} \right) + 2\sum_{\ell=1}^{\lfloor r/2 \rfloor} B(\ell,k,r)$$

and

$$4\left\lfloor \frac{r}{2} \right\rfloor \sqrt{d} \left(\cos \frac{\pi}{k+1} + b - \cos \frac{\pi}{k} \right) < E(T(d,k,r)) - rE(B_{d,k}) + (r-1)E(S_k)$$

whenever r is odd and k is odd.

Example.

d	k	r	E(T(d,k,r))	lower bound	upper bound
2	5	4	105.00	97.59	114.74
2	4	3	29.78	24.90	34.21
4	4	2	130.25	124.18	137.36
4	5	3	861.58	856.63	868.31

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