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Chemical trees minimizing energy and Hosoya index

Clemens Heuberger · Stephan G. Wagner

Abstract   The energy of a molecular graph is a popular parameter that is defined as the sum of the absolute values of a graph's eigenvalues. It is well known that the energy is related to the matching polynomial and thus also to the Hosoya index via a certain Coulson integral. It is quite a natural problem to minimize the energy of trees with bounded maximum degree—clearly, the case of maximum degree 4 (so-called chemical trees) is the most important one. We will show that the trees with given maximum degree that minimize the energy are the same that have been shown previously to minimize the Hosoya index and maximize the Merrifield-Simmons index, thus also proving a conjecture due to Fischermann et al. Finally, we show that the minimum energy grows linearly with the size of the trees, with explicitly computable growth constants that only depend on the maximum degree.

1 Introduction and statement of results

The energy is a graph parameter stemming from the Hückel molecular orbital (HMO) approximation for the total π-electron energy, see [4, 5]. It is defined as the sum of the absolute values of all eigenvalues of a graph: if $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ denotes the spectrum of a graph G (i.e. the spectrum of its adjacency matrix), one has

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$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

For more information about the chemical importance of the energy as well as important properties, we refer to the book [6] and the survey article [5]. It is known that there are many interesting relations between the spectrum and matchings in the case of trees. This is due to the fact that the characteristic polynomial $\phi(T, x) = \det(xI - A(T))$, where $A(T)$ denotes the adjacency matrix of a tree T and I the identity matrix, can be expressed [1] as

$$\phi(T, x) = \sum_{k \geq 0} (-1)^k m(T, k) x^{n-2k}, \tag{1}$$

where $m(T, k)$ denotes the number of matchings of T of cardinality k. It follows from this representation that the energy can actually be computed by means of the Coulson integral [6]

$$E(T) = \frac{2}{\pi} \int_0^\infty x^{-2} \log \left(\sum_k m(T, k) x^{2k} \right) dx. \tag{2}$$

This connection to matchings has been used in various instances (the first one being about 30 years ago, see [3]) to determine the extremal values of the energy within certain classes of graphs (trees or graphs that are closely related to trees, such as unicyclic graphs or generally graphs with a bounded number of cycles—see [13–16, 19, 20, 22, 24]). We mention, for instance, the recent papers of Yan and Ye [23] and of Zhou and Li [28], where trees with prescribed diameter minimizing the energy are characterized. In [25] and [26], trees with a given number of leaves (pendent vertices) are studied. An earlier example is the article by Zhang and Li [27], where trees with a perfect matching are studied (see also [17]). For further recent progress, the reader is referred to [7, 18].

For obvious reasons, it is also a natural problem to study *chemical trees* (i.e., trees with maximum degree ≤ 4) and generally trees with bounded maximum degree. Fischermann et al. [2] noticed that the chemical trees minimizing the energy agree with those minimizing the Hosoya index (i.e., the total number of matchings, see [12]) for a small number of vertices. Indeed, we will show that this is always the case and also holds for arbitrary given maximum degree. The resulting trees have also been shown to maximize the Merrifield-Simmons index (i.e., the total number of independent vertex subsets, see [21]) in an earlier paper by the authors [9]. We will show that essentially the same method can be used again. In view of the representation (2), it is sufficient to minimize the polynomial
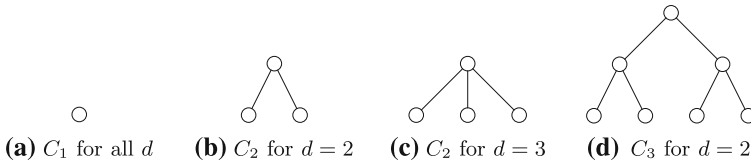
$$M(T, x) = \sum_k m(T, k) x^k$$

(a) C_1 for all d **(b)** C_2 for $d = 2$ **(c)** C_2 for $d = 3$ **(d)** C_3 for $d = 2$

Fig. 1 Complete d-ary trees

for all positive values of x, cf. [3]. Surprisingly, it turns out that the result of this minimization problem does not depend on x.

In order to state our result, we use the notion of *complete d-ary trees*: the complete d-ary tree of height $h - 1$ is denoted by C_h, i.e., C_1 is a single vertex and C_h has d branches $C_{h-1},\ldots,C_{h-1}$, cf. Fig. 1. It is convenient to set C_0 to be the empty graph.

Let $\mathcal{T}_{n,d}$ be the set of all trees with n vertices and maximum degree $\leq d + 1$. We define a special tree $T_{n,d}^*$ as follows (see also [9]):

Definition 1.1 $T_{n,d}^*$ is the tree with n vertices that can be decomposed as
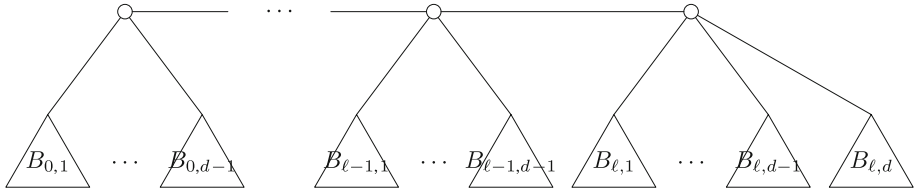
with $B_{k,1},\ldots,B_{k,d-1} \in \{C_k, C_{k+2}\}$ for $0 \leq k < \ell$ and either $B_{\ell,1} = \cdots = B_{\ell,d} = C_{\ell-1}$ or $B_{\ell,1} = \cdots = B_{\ell,d} = C_\ell$ or $B_{\ell,1},\ldots, B_{\ell,d} \in \{C_\ell, C_{\ell+1}, C_{\ell+2}\}$, where at least two of $B_{\ell,1},\ldots,B_{\ell,d}$ equal $C_{\ell+1}$. This representation is unique, and one has the "digital expansion"

$$(d - 1)n + 1 = \sum_{k=0}^{\ell} a_k d^k, \tag{3}$$

where $a_k = (d - 1)(1 + (d + 1)r_k)$ and $0 \leq r_k \leq d - 1$ is the number of $B_{k,i}$ that are isomorphic to C_{k+2} for $k < \ell$, and

- $a_\ell = 1$ if $B_{\ell,1} = \cdots = B_{\ell,d} = C_{\ell-1}$,
- $a_\ell = d$ if $B_{\ell,1} = \cdots = B_{\ell,d} = C_\ell$,
- or otherwise $a_\ell = d + (d - 1)q_\ell + (d^2 - 1)r_\ell$, where $q_\ell \geq 2$ is the number of $B_{\ell,i}$ that are isomorphic to $C_{\ell+1}$ and r_ℓ the number of $B_{\ell,i}$ that are isomorphic to $C_{\ell+2}$.

As examples, the trees $T_{n,d}^*$ for $n = 69$ and $d = 2, 3, 4$ are shown in Figs. 2–5. Further details on the algorithmic construction of $T_{n,d}^*$ for given n and d are discussed in [10].
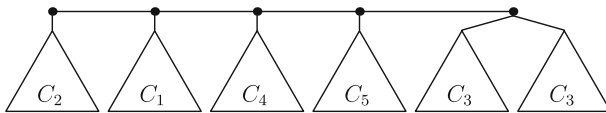
The tree $T_{n,d}^*$ has already been shown to minimize the Hosoya index and maximize the Merrifield-Simmons index over $\mathcal{T}_{n,d}$ [9]. In the present paper, we will prove the following result:
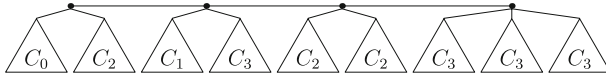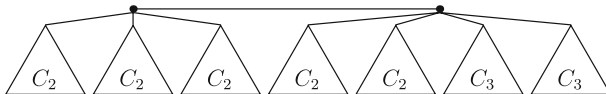
Fig. 2 $T^*_{69,3}$ in the decomposition described in Theorem 1. An explicit version is shown in Fig. 3
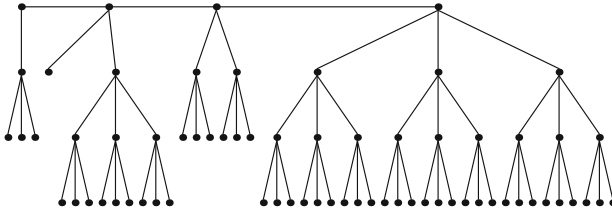
Fig. 3 $T^*_{69,3}$, explicit version

Fig. 4 $T^*_{69,2}$

Fig. 5 $T^*_{69,4}$

Proposition 1.2 *Let n and d be positive integers and x > 0. Then $T^*_{n,d}$ is the unique (up to isomorphism) tree in $\mathcal{T}_{n,d}$ that minimizes $M(T, x)$.*   □

Note that the Hosoya index is exactly $M(T, 1)$, and so it is a trivial corollary that $T^*_{n,d}$ minimizes the Hosoya index. Our main theorem is another immediate consequence that follows from (2):

Theorem 1 *Let n and d be positive integers. Then $T^*_{n,d}$ is the unique (up to isomorphism) tree in $\mathcal{T}_{n,d}$ that minimizes the energy.*

In our final section, we will study the asymptotic behavior of the minimum energy:

Theorem 2 *The energy of $T^*_{n,d}$ is asymptotically*

$$E(T^*_{n,d}) = \alpha_d n + O(\log n),$$

where

$$
\alpha_d = 2\sqrt{d}(d-1)^2 \left(\sum_{\substack{j \geq 1 \\ j \equiv 0 \ \text{mod } 2}} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) + \sum_{\substack{j \geq 1 \\ j \equiv 1 \ \text{mod } 2}} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right)
\tag{4}
$$

is a constant that only depends on d.

2 Recursive formulæ for rooted trees

Let $x > 0$ be fixed. A typical way to determine $M(T, x)$ recursively is the formula

$$
M(T, x) = M(T \backslash e, x) + x M(T \backslash \{v, w\}, x)
\tag{5}
$$

that holds for any edge $e = vw$ of T, cf. [3]. For our purposes, it will be useful to introduce two auxiliary quantities first. We fix a root r of T, and we define $m_1(T, k)$ to be the number of matchings of cardinality k covering the root and $m_0(T, k)$ to be the number of matchings of cardinality k not covering the root.

Furthermore, we write $M_j(T, x) = \sum_k m_j(T, k) x^k$ for $j \in \{0, 1\}$. Obviously, we have $M(T, x) = M_0(T, x) + M_1(T, x)$. The ratio

$$
\tau(T, x) = \frac{M_0(T, x)}{M(T, x)}
\tag{6}
$$

will be an important auxiliary quantity in our proofs. The following lemma summarizes important properties of all these quantities, for which we will provide short self-contained proofs as well (following the ideas used to prove (5)).

Lemma 2.1 *Let $T_1, \ldots, T_\ell$ be the branches of the rooted tree T. Then the following recursive formulæ hold:*

$$
M_0(T, x) = \prod_{i=1}^{\ell} M(T_i, x),
\tag{7}
$$

$$
M_1(T, x) = x \sum_{i=1}^{\ell} M_0(T_i, x) \prod_{\substack{j=1 \\ j \neq i}}^{\ell} M(T_j, x),
\tag{8}
$$

$$
\tau(T, x) = \frac{1}{1 + x \sum_{i=1}^{\ell} \tau(T_i, x)}.
\tag{9}
$$

Proof A matching not covering the root corresponds to a selection of an arbitrary matching in each branch. If the matching of T is required to have cardinality k, the cardinalities of the corresponding matchings in the branches must add up to k. This is exactly the coefficient of x^k in the product $\prod_{i=1}^{\ell} M(T_i, x)$. This proves (7).

Every matching of T covering the root contains exactly one edge between the root and some branch T_i. In this branch, a matching not covering the root of T_i may be chosen, in all other branches, arbitrary matchings are allowed. The cardinality of the matching of T is then the sum of the cardinalities of the matchings in the branches plus one for the edge incident to the root. This yields (8).

Finally, (9) is an immediate consequence of (6), (7) and (8).   □

In the following, we will fix a positive integer d and consider only trees whose maximum degree is $\leq d + 1$. First of all, we study the behavior of the sequence $\tau(C_h, x)$. It is convenient to set $M_0(C_0, x) = 0$ and $M_1(C_0, x) = 1$ for the polynomials associated to the empty tree. Note that this choice allows adding empty branches without disturbing the recursive formulæ (7), (8), (9). Then (9) translates into a recursion for $\tau(C_h, k)$ as follows:

$$\tau(C_0, x) = 0, \quad \tau(C_1, x) = 1, \quad \tau(C_h, x) = \frac{1}{1 + dx\tau(C_{h-1}, x)}.$$

It is an easy exercise to prove the following explicit formula for $\tau(C_h, x)$ by means of induction:

Lemma 2.2 *For every $x > 0$, we have*

$$\tau(C_h, x) = \frac{\left(\frac{1+\sqrt{1+4dx}}{2}\right)^h - \left(\frac{1-\sqrt{1+4dx}}{2}\right)^h}{\left(\frac{1+\sqrt{1+4dx}}{2}\right)^{h+1} - \left(\frac{1-\sqrt{1+4dx}}{2}\right)^{h+1}}.$$

Now, the limit behavior of $\tau(C_h, x)$ for positive x follows immediately.

Lemma 2.3 *For every $x > 0$, the subsequence $\tau(C_{2h}, x)$ is strictly increasing, whereas the subsequence $\tau(C_{2h+1}, x)$ is strictly decreasing. Both subsequences converge to the same limit $\frac{2}{1+\sqrt{1+4dx}}$ and we have*

$$0 = \tau(C_0, x) < \tau(C_2, x) < \cdots < \frac{2}{1 + \sqrt{1+4dx}} < \cdots < \tau(C_3, x) < \tau(C_1, x) = 1.$$
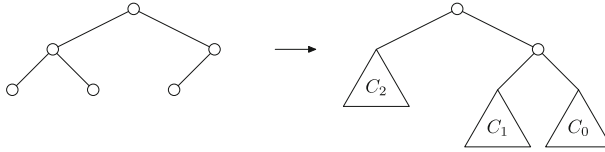
From this point on, the method of [9], in particular Sect. 5, can be applied. It suffices to replace d by dx at certain points of the proof. For the sake of completeness, we state the relevant auxiliary results.

Lemma 2.4 *Let T be a rooted tree and $x > 0$. Then*

$$\frac{1}{dx + 1} \leq \tau(T, x) \leq 1,$$

unless T is empty, where $\tau(T, x) = 0$.

Proof To prove this lemma, use induction and Lemma 2.1.   □

Fig. 6 Reduction to the outline graph ($d = 2$)

Definition 2.5 Let T be a possibly rooted tree. Then we construct the *outline graph* of T by replacing all maximal subtrees isomorphic to some C_k, $k \geq 0$, by a special leaf C_k. In this process, we attach $(d + 1 - r)$ leaves C_0 to internal nodes (non-leaves and non-root) of degree r with $2 \leq r \leq d$. If T is a rooted tree with a root of degree r ($1 \leq r \leq d$), then we also attach $d - r$ leaves C_0 to it.

The construction ensures that the outline graph of a rooted tree is a rooted d-ary tree, and that the outline graph of an arbitrary tree of maximum degree $\leq d + 1$ has only vertices of degree 1 and $d + 1$. An example is shown in Fig. 6. The outline of a rooted tree C_k is just the rooted tree consisting of the single leaf C_k.

If enough information on the outline of a rooted tree is available, we can determine it from its $\tau(T, x)$-value.

Lemma 2.6 *Let $j \geq 0$ be an integer and T be a rooted tree whose outline does not contain any C_k for $0 \leq k \leq j - 3$ and $x > 0$. If*

$$j \text{ is odd and } \tau(C_j, x) \leq \tau(T, x)$$

or

$$j \text{ is even and } \tau(T, x) \leq \tau(C_j, x),$$

then $T \in \{C_{j-2}, C_j\}$.

Proof The inductive proof is analogous to that of [9, Lemma 3.4], the only difference being the fact that here, sums are considered instead of products.   □

3 Minimal trees with respect to x

We say that T is a minimal tree with respect to some $x > 0$, if it minimizes $M(T, x)$ among all trees in $\mathcal{T}_{n,d}$.

The key lemma is an exchange lemma which gives a local optimality criterion.

Lemma 3.1 *Let $x > 0$ and let T be a minimal tree with respect to x. If there are (possibly empty) rooted trees $L_1, \ldots, L_d$, $R_1, \ldots, R_d$ and a tree T_0 such that T can be decomposed as*
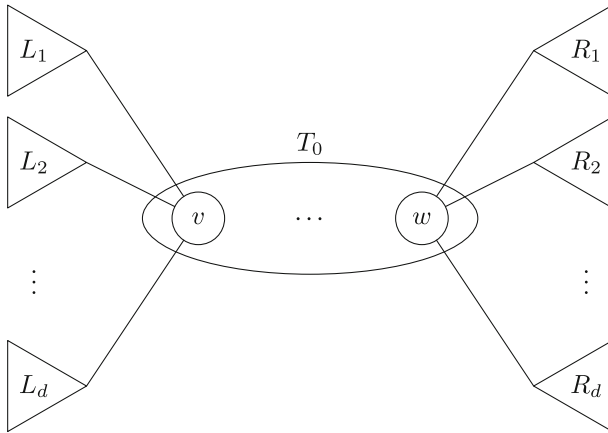
and such that $\tau(L_1, x) < \tau(R_1, x)$ (after appropriate reordering of the L_i's and the R_i's), then

$$\max\{\tau(L_i, x) : 1 \leq i \leq d\} \leq \min\{\tau(R_i, x) : 1 \leq i \leq d\}.$$

Proof We need four auxiliary quantities:

- $m_{00}(T_0, k)$: number of matchings of T_0 of cardinality k where neither v nor w is covered.
- $m_{10}(T_0, k)$: number of matchings of T_0 of cardinality k where v is covered, but w is not.
- $m_{01}(T_0, k)$: number of matchings of T_0 of cardinality k where w is covered, but v is not.
- $m_{11}(T_0, k)$: number of matchings of T_0 of cardinality k where both v and w are covered.

The corresponding polynomials are denoted by $M_{ij}(T_0, x) = \sum_k m_{ij}(T_0, k)x^k$. Define

$$\begin{aligned}
&G(L_1, \ldots, L_d, R_1, \ldots, R_d; x) \\
&:= M_{00}(T_0, x)\left(1 + x\sum_{i=1}^{d}\tau(L_i, x)\right)\left(1 + x\sum_{i=1}^{d}\tau(R_i, x)\right) \\
&\quad + M_{10}(T_0, x)\left(1 + x\sum_{i=1}^{d}\tau(R_i, x)\right) \\
&\quad + M_{01}(T_0, x)\left(1 + x\sum_{i=1}^{d}\tau(L_i, x)\right) + M_{11}(T_0, x).
\end{aligned}$$

Then it is easily seen that

$$M(T, x) = G(L_1, \ldots, L_d, R_1, \ldots, R_d; x) \prod_{i=1}^{d} M(L_i, x) \prod_{i=1}^{d} M(R_i, x).$$

In view of the minimality of $M(T, x)$, we must have

$$G(L_1, \ldots, L_d, R_1, \ldots, R_d; x) \leq G(\pi(L_1), \ldots, \pi(L_d), \pi(R_1), \ldots, \pi(R_d); x)$$

for all permutations π of $\{L_1, \ldots, L_d, R_1, \ldots, R_d\}$. Ignoring the assumption $\tau(L_1, x) < \tau(R_1, x)$ for the moment, we see that the minimum of the first summand among all possible permutations is attained if

$$\max\{\tau(L_i, x) : i = 1, \ldots, d\} \leq \min\{\tau(R_i, x) : i = 1, \ldots, d\} \text{ or} \quad (10)$$
$$\min\{\tau(L_i, x) : i = 1, \ldots, d\} \geq \max\{\tau(R_i, x) : i = 1, \ldots, d\}$$

by standard arguments (note that the sum of the two factors does not depend on the permutation). The sum of the second and the third summand is minimized if $\max\{\tau(L_i, x) : i = 1, \ldots, d\} \leq \min\{\tau(R_i, x) : i = 1, \ldots, d\}$ in the case $M_{10}(T_0, x) \leq M_{01}(T_0, x)$ and is minimized if $\min\{\tau(L_i, x) : i = 1, \ldots, d\} \geq \max\{\tau(R_i, x) : i = 1, \ldots, d\}$ in the case that $M_{10}(T_0, x) \geq M_{01}(T_0, x)$. Therefore, the minimality of G yields (10). The assumption $\tau(L_1, x) < \tau(R_1, x)$ implies the first possibility. □

The remaining steps of the proof in [9] do not depend on the particular recursions any more, they only depend on the monotonicity properties in Lemma 2.3 and Lemma 2.6 as well as the local optimality criterion in Lemma 3.1. The only difference is that all inequalities have to be reversed (and $\rho(T)$ has to be replaced by $\tau(T, x)$). Thus the basis of the final induction can be formulated as follows.

Lemma 3.2 *Let T be a minimal tree with respect to $x > 0$ and let j be the least nonnegative integer such that the outline graph of T contains a C_j. Then the outline graph of T contains C_j at most $(d - 1)$ times and there is a vertex v of the outline graph of T which is adjacent to all copies of C_j in the outline graph of T.*

Proof Analogous to the proof of [9, Lemma 4.3]. □

The inductive step can be formulated as follows.

Lemma 3.3 *Let $x > 0$, T be a minimal tree with respect to x, k be a nonnegative integer and assume that the outline graph of T can be decomposed as*

for some rooted trees L_k (possibly empty) and R_k with

$$k \text{ is even and } \tau(C_k, x) < \tau(L_k, x) < \tau(C_{k+2}, x)$$

or

$$k \text{ is odd and } \tau(C_{k+2}, x) < \tau(L_k, x) < \tau(C_k, x)$$
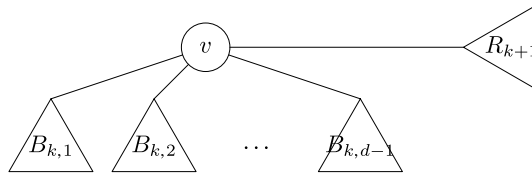
or

$$L_k = C_k.$$

Assume that R_k is non-empty and the outline of R_k does not contain any C_ℓ with $\ell < k$.

Then exactly one of the following assertions is true:

1. $R_k \in \{C_k, C_{k+1}, C_{k+3}\}$,
2. R_k consists of d branches $C_{k+1}, C_{k+1}, C_{\ell_3},..., C_{\ell_d}$ with $\ell_i \in \{k, k+1, k+2\}$ for $3 \leq i \leq d$,
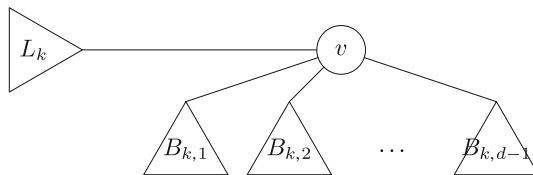3. the outline of R_k can be decomposed as

for $B_{k,1},..., B_{k,d-1} \in \{C_k, C_{k+2}\}$ and a non-empty rooted tree R_{k+1} whose outline does not contain any C_ℓ for $\ell \leq k$. Furthermore,

$$k \text{ is even and } \tau(C_{k+3}, x) < \tau(L_{k+1}, x) < \tau(C_{k+1}, x)$$

or

$$k \text{ is odd and } \tau(C_{k+1}, x) < \tau(L_{k+1}, x) < \tau(C_{k+3}, x)$$

where L_{k+1} is defined as follows:

Proof Analogous to the proof of [9, Lemma 4.4].   □

Repeated application of Lemma 3.3 now yields Proposition 1.2 and thus also our main theorem.

[*Proof of Proposition* 1.2] Analogous to the proof of [9, Theorem 1].   □

4 The value of the minimum energy

Since the extremal trees are described in terms of complete d-ary trees, we have to study the energy of these trees first. Note that, in view of (7) and the definition of $\tau(M, x)$, we have

$$M(C_h, x) = \frac{1}{\tau(C_h, x)} \cdot M(C_{h-1}, x)^d.$$

Iterating this equation yields

$$M(C_h, x) = \prod_{j=1}^{h} \tau(C_j, x)^{-d^{h-j}},$$

and in view of Lemma 2.2 this gives us the explicit formula

$$M(C_h, x) = \prod_{j=1}^{h} \left(\frac{Q_{j+1}(x)}{Q_j(x)} \right)^{d^{h-j}},$$

where

$$Q_j(x) := \frac{u(x)^j - v(x)^j}{u(x) - v(x)},$$

$$u(x) := \frac{1 + \sqrt{1 + 4dx}}{2},$$

$$v(x) := \frac{1 - \sqrt{1 + 4dx}}{2}.$$

The denominator $u(x) - v(x)$ has been introduced such that $Q_j(x)$ is always a polynomial: Indeed, the recursion

$$Q_1(x) \equiv 1, \quad Q_2(x) \equiv 1, \quad Q_j(x) = Q_{j-1}(x) + dx Q_{j-2}(x)$$

holds, and it follows by induction that Q_j is a polynomial of degree $\lfloor (j - 1)/2 \rfloor$. It should be noted that Q is closely related to the so-called Fibonacci polynomials (see [11]). Now we have

$$M(C_h, x) = Q_{h+1}(x) Q_1(x)^{-d^{h-1}} \prod_{j=2}^{h} Q_j(x)^{d^{h+1-j}} \prod_{j=2}^{h} Q_j(x)^{-d^{h-j}}$$

$$= Q_{h+1}(x) \prod_{j=1}^{h} Q_j(x)^{(d-1)d^{h-j}},$$

where the fact that $Q_1(x) = 1$ has been used. It turns out that the zeros of Q_j can be explicitly computed. If $Q_j(x) = 0$, then $u(x)^j = v(x)^j$, and so

$$\frac{u(x)}{v(x)} = \frac{1 + \sqrt{1 + 4dx}}{1 - \sqrt{1 + 4dx}}$$

has to be a jth root of unity ζ. Then,

$$x = -\frac{\zeta}{d(1 + \zeta)^2} = -\frac{1}{2d(1 + \text{Re}(\zeta))}.$$

Thus, x has to be of the form

$$x = -\frac{1}{2d \left(1 + \cos \frac{2k\pi}{j}\right)}$$

for some $0 \le k < \frac{j}{2}$. However, note that $x = -\frac{1}{4d}$ is also a zero of the denominator $u(x) - v(x) = \sqrt{1 + 4dx}$, and that there are no double zeros, since the derivative is given by

$$\frac{d}{dx}\left(u(x)^j - v(x)^j\right) = \frac{jd}{\sqrt{1 + 4dx}}\left(u(x)^{j-1} + v(x)^{j-1}\right),$$

which cannot be 0 if $u(x) = \zeta v(x)$ for a jth root of unity $\zeta \ne -1$. Hence, the zeros of Q_j are precisely the numbers

$$-\frac{1}{2d \left(1 + \cos \frac{2k\pi}{j}\right)}, \quad k = 1, 2, \ldots, \left\lfloor \frac{j-1}{2} \right\rfloor,$$

and it follows from (1) that the characteristic polynomial $\phi(C_h, x)$ can be written as

$$\phi(C_h, x) = x^n M(C_h, -x^{-2}) = x^n Q_{h+1}(-x^{-2}) \prod_{j=1}^{h} Q_j(-x^{-2})^{(d-1)d^{h-j}}.$$

Hence, the nonzero eigenvalues of C_h are

$$\pm\sqrt{2d \left(1 + \cos \frac{2k\pi}{j}\right)} = \pm 2\sqrt{d} \cos \frac{k\pi}{j}, \quad k = 1, 2, \ldots, \left\lfloor \frac{j-1}{2} \right\rfloor,$$

with multiplicity $(d-1)d^{h-j}$ for $j = 1, 2, \ldots, h$ and multiplicity 1 for $j = h + 1$. If follows that the energy of C_h is given by

$$E(C_h) = \left(\sum_{j=1}^{h} (d-1)d^{h-j} \sum_{k=1}^{\lfloor (j-1)/2 \rfloor} 4\sqrt{d} \cos \frac{k\pi}{j} \right) + \sum_{k=1}^{\lfloor h/2 \rfloor} 4\sqrt{d} \cos \frac{k\pi}{h+1}.$$

Noticing that

$$\sum_{k=1}^{\lfloor (j-1)/2 \rfloor} \cos \frac{k\pi}{j} = \begin{cases} \frac{1}{2} \left(\cot \frac{\pi}{2j} - 1 \right) & j \equiv 0 \mod 2, \\ \frac{1}{2} \left(\csc \frac{\pi}{2j} - 1 \right) & j \equiv 1 \mod 2, \end{cases}$$

this reduces to

$$E(C_h) = 2\sqrt{d}(d-1) \left(\sum_{\substack{j=1 \\ j \equiv 0 \mod 2}}^{h} d^{h-j} \left(\cot \frac{\pi}{2j} - 1 \right) + \sum_{\substack{j=1 \\ j \equiv 1 \mod 2}}^{h} d^{h-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right)$$

$$+ \begin{cases} 2\sqrt{d} \left(\csc \frac{\pi}{2(h+1)} - 1 \right) & h \equiv 0 \mod 2, \\ 2\sqrt{d} \left(\cot \frac{\pi}{2(h+1)} - 1 \right) & h \equiv 1 \mod 2. \end{cases}$$

Next, we determine the asymptotic behavior of the energy of C_h:

Lemma 4.1 *The energy of a complete d-ary tree C_h satisfies*

$$E(C_h) = \alpha_d |C_h| + O(1),$$

where $|C_h|$ denotes the number of vertices of C_h and α_d is given by (4).

Proof Note that $|C_h| = \frac{d^h - 1}{d-1} = \frac{d^h}{d-1} + O(1)$ and $\cot \frac{\pi}{2j} = \frac{2j}{\pi} + O(1)$, $\csc \frac{\pi}{2j} = \frac{2j}{\pi} + O(1)$, so that

$$E(C_h) = 2\sqrt{d}(d-1)d^h \left(\sum_{\substack{j=1 \\ j \equiv 0 \mod 2}}^{h} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) \right.$$

$$\left. + \sum_{\substack{j=1 \\ j \equiv 1 \mod 2}}^{h} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right) + \frac{4\sqrt{d}h}{\pi} + O(1)$$

$$= \alpha_d |C_h| - 2\sqrt{d}(d-1)d^h \left(\sum_{\substack{j > h \\ j \equiv 0 \mod 2}} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) \right)$$

$$+ \sum_{\substack{j>h \\ j\equiv 1 \mod 2}} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \Bigg) + \frac{4\sqrt{d}h}{\pi} + O(1)$$

$$= \alpha_d |C_h| - 2\sqrt{d}(d-1)d^h \sum_{j>h} d^{-j} \left(\frac{2j}{\pi} + O(1) \right) + \frac{4\sqrt{d}h}{\pi} + O(1)$$

$$= \alpha_d |C_h| - 2\sqrt{d}(d-1)d^h \left(\frac{2hd^{-h}}{(d-1)\pi} + O(d^{-h}) \right) + \frac{4\sqrt{d}h}{\pi} + O(1)$$

$$= \alpha_d |C_h| + O(1),$$

as claimed.   □

Now, we are able to prove our main asymptotic result:

Proof of Theorem Using the decomposition of $T_{n,d}^*$ as shown in Definition 1.1, we note that

$$\left(\prod_{k=0}^{\ell-1} \prod_{j=1}^{d-1} M(B_{k,j}, x) \right) \left(\prod_{j=1}^{d} M(B_{\ell,j}, x) \right) \le M(T_{n,d}^*, x)$$

$$\le \left(\prod_{k=0}^{\ell-1} \prod_{j=1}^{d-1} M(B_{k,j}, x) \right) \left(\prod_{j=1}^{d} M(B_{\ell,j}, x) \right) (1+x)^{d(\ell+1)}$$

for arbitrary $x > 0$, since every matching in the union $\bigcup_k \bigcup_j B_{k,j}$ is also a matching in $T_{n,d}^*$, whereas every matching of $T_{n,d}^*$ consists of a matching in $\bigcup_k \bigcup_j B_{k,j}$ and a subset of the remaining $\le d(\ell+1)$ edges. Making use of (2) once again, this implies that

$$\sum_{k=0}^{\ell-1} \sum_{j=1}^{d-1} E(B_{k,j}) + \sum_{j=1}^{d} E(B_{\ell,j}) \le E(T_{n,d}^*) \le \sum_{k=0}^{\ell-1} \sum_{j=1}^{d-1} E(B_{k,j})$$

$$+ \sum_{j=1}^{d} E(B_{\ell,j}) + \frac{2}{\pi} d(\ell+1) \int_0^\infty x^{-2} \log(1+x^2)\,dx.$$

Since $\int_0^\infty x^{-2} \log(1+x^2)\,dx = \pi$, this implies that

$$E(T_{n,d}^*) = \sum_{k=0}^{\ell-1} \sum_{j=1}^{d-1} E(B_{k,j}) + \sum_{j=1}^{d} E(B_{\ell,j}) + O(\ell)$$

$$= \sum_{k=0}^{\ell-1} \sum_{j=1}^{d-1} \left(\alpha_d |B_{k,j}| + O(1) \right) + \sum_{j=1}^{d} \left(\alpha_d |B_{\ell,j}| + O(1) \right) + O(\ell)$$

$$= \alpha_d \left(\sum_{k=0}^{\ell-1} \sum_{j=1}^{d-1} |B_{k,j}| + \sum_{j=1}^{d} |B_{\ell,j}| \right) + O(\ell)$$

$$= \alpha_d (|T_{n,d}^*| - O(\ell)) + O(\ell) = \alpha_d n + O(\ell).$$

It is not difficult to see that $\ell = O(\log n)$ (this follows from (3), see [8] for a detailed analysis), and so we finally have

$$E(T_{n,d}^*) = \alpha_d n + O(\log n),$$

which finishes the proof.   □

The following table shows some numerical values of the constants α_d:

d	α_d
2	1.102947505597
3	0.970541979946
4	0.874794345784
5	0.802215758706
6	0.744941364903
7	0.698315075830
8	0.659425329682
9	0.626356806404
10	0.597794680849
20	0.434553264777
50	0.279574397741
100	0.198836515295

5 Conclusion

In this paper, we were able to prove that the trees with a given number n of vertices and given maximum degree $d + 1$ that minimize the energy are exactly the trees $T_{n,d}^*$ that were shown earlier to minimize the Hosoya index and maximize the Merrifield-Simmons index (which was conjectured and proven for a small number of vertices by Fischermann et al. [2]). The extremal trees are unique up to isomorphism and can be described in terms of complete d-ary trees (as seen in Definition 1.1).

The fact that these trees minimize the energy and the Hosoya index is actually a mere corollary of the more general result (Proposition 1.2) that they minimize the matching polynomial $M(T, x)$ for arbitrary positive x. The main theorem (Theorem 1) is then a consequence of the well-known representation of the energy as a Coulson integral. Indeed, it is believable that even all coefficients of the matching polynomial are minimized (i.e., $T_{n,d}^*$ is also the smallest element with respect to the partial order $\prec$ introduced in [3]: for two trees T_1 and T_2, $T_1 \prec T_2$ if and only if $m(T_1, k) \leq m(T_2, k)$ for all k), even though this is probably much more difficult to prove. The trees $T_{n,d}^*$ might also be extremal with respect to other graph parameters similar to the energy, the Hosoya index and the Merrifield-Simmons index.

Finally, it is also possible to describe the asymptotic behavior of the energy of the extremal trees $T_{n,d}^*$ quite precisely. The minimum energy of a tree with n vertices and maximum degree $d + 1$ grows linearly in n and is approximately equal to $\alpha_d n$, where α_d is an explicitly computable constant (given in (4)).

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