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ON THE NUMBER OF WALKS IN TREES

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Abstract

Let W_k be the number of walks of length k in a graph G, and put $\Delta_k := W_{k+1}\,W_{k-1} - W_k^2$. In recent work, it was shown that exactly one of the following four alternatives holds:

- $\Delta_1 \geq 0$ and $\Delta_k = 0$ for all $k = 2, 3, \ldots$ in which case G is said to be harmonic,
- $\Delta_{2k-1} > 0$ and $\Delta_{2k} = 0$ for all $k = 1, 2, \ldots$ in which case G is said to be almost harmonic,
- $\Delta_{2k-1} > 0$ for all $k = 1, 2, \ldots$ and $\Delta_{2k} > 0$ for all sufficiently large k in which case G is said to be superharmonic, and
- $\Delta_{2k-1} > 0$ for all $k = 1, 2, \ldots$ and $\Delta_{2k} < 0$ for all sufficiently large k in which case G is said to be subharmonic.

We examined all trees (up to isomorphism) with up to 18 vertices and determined how many of them belong to each of the four classes specified above. In agreement with a previously established result (cf. S. Grünewald, Harmonic Trees, *Appl. Math. Lett.*, to appear) according to which a harmonic tree with at least 3 vertices always has exactly one vertex of degree $a^2 - a + 1$ all of whose neighbours have degree a while all other vertices are leaves (for some $a \in \mathbb{N}_{\geq 2}$), exactly three (with 1, 2, and 7 vertices, respectively) of those trees turned out to be harmonic, no one is almost harmonic, 11 are superharmonic (of which the smallest has 12 vertices), and all others — some 99.994% of all trees examined — are subharmonic.

1 Introduction

1.1 Walks in Graphs

Given a finite simple graph $G = (V, E)$ with vertex set $V = V_G$ and edge set $E = E_G \subseteq \binom{V}{2}$, a *walk* of length k in G is a $(k+1)$-tuple $v_0, v_1, \ldots, v_k$ of vertices of G with $\{v_{i-1}, v_i\} \in E$ for all $i = 1, 2, \ldots, k$. Such a walk is said to start at vertex v_0 and to end at vertex v_k.

Walks are not required to consist of mutually distinct vertices, only. In particular, if $v_0 = v_k$, then $v_0, v_1, \ldots, v_k$ is a *self-returning* walk (of length k).

The number of walks of length k of G starting at a given vertex v is denoted by $d_k(v)$ and the number of all walks in G of length k by $W_k = W_k(G)$. Thus, $d_1(v)$ is nothing but the degree $d(v) = d_G(v)$ of v, and one has $W_0 = \#V$, $W_1 = 2\#E$, and

$$d_{k+1}(v) = \sum_{w \in N(v)} d_k(w) \text{ as well as } W_k = \sum_{v \in V} d_k(v)$$

for every $k \in \mathbb{N}_0$.

Next, let

$$A = A_G = (a_{vw})_{v,w \in V}$$

denote the *adjacency* matrix of G. Then the powers

$$A^k = (a_{vw}^{(k)})_{v,w \in V}$$

of A count the number of walks in G. Indeed, the entry $a_{vw}^{(k)}$ coincides with the number $W_k(v, w)$ of walks of length k in the graph G with start vertex v and end vertex w:

$$a_{vw}^{(k)} = W_k(v, w) \ . \tag{1}$$

1.2 Walks in Molecular Graphs

This elementary result has fascinated theoretical chemists for quite some time. In early work, the corollary that the trace of A^k coincides with the total number of self-returning walks of length k was applied in the theory of total π-electron energy [1]. Eventually this direction of research was continued in numerous other studies, see [2–8] and the references cited therein. Another chemical application was put forward in [9] where atomic environments were characterized by means of the sequences $a_{rr}^{(k)}$, $k \in \mathbb{N} := \{1, 2, \ldots\}$. Also this direction of research was extensively pursued, see [10–14] and the references cited therein. Somewhat later, the attention of theoretical chemists turned to the total number of walks [14, 15]. The main results in this direction were obtained by Gerta and Christoph Rücker [16–21]. They introduced the concept of the *total walk count* defined by

$$twc = twc_G := \sum_{k=0}^{\#V-1} W_k$$

and demonstrated how this number can be used in QSPR and QSAR studies [16,18–20].

Clearly, Eq. (1) implies

$$W_k = \sum_{v,w \in V} W_k(v,w) = \sum_{v,w \in V} a_{vw}^{(k)}, \tag{2}$$

a formula that can be used for easy computer-aided calculation of W_k. While studying the mathematical properties of W_k [20] in detail, it was observed that the fine structure of the k-dependence of W_k is, in a concealed manner, determined by the parity of k. In particular, whereas $W_{k+1} - W_k$ is always greater than $W_k - W_{k-1}$, this is not always true when, instead of W_k, we consider its logarithm. Indeed, while the signs of the quantities $(\log W_{k+1}(G) - \log W_k(G)) - (\log W_k(G) - \log W_{k-1}(G))$ or, equivalently, those of the quantities

$$\Delta_k = \Delta_k(G) := W_{k+1}(G)\, W_{k-1}(G) - W_k(G)^2 \quad (k \in \mathbb{N}) \tag{3}$$

appear to exhibit some regularity, these signs cannot easily be predicted in general from the value of k and just some simple standard properties of and/or basic numerical quantities attached to a graph G. Yet, spectral graph theory [22] proved to be a useful tool in the study of Δ_k, and some important conclusions regarding the sign of $\Delta_k(G)$ could be obtained by using graph eigenvalues and eigenvectors.

1.3 Walks and the Spectrum of Graphs

Continuing with our notation, let

$$U_\mu = U_\mu(G) := \{u \in \mathbb{R}^V \,|\, Au = \mu u\} \quad (\mu \in \mathbb{R})$$

denote the space of eigenvectors of $A = A_G$ with eigenvalue μ, let

$$\mathrm{spec}(G) := \mathrm{spec}(A) := \{\mu \in \mathbb{R} : \dim U_\mu > 0\}$$

denote the *spectrum* of G, consider the canonical decomposition

$$j = \sum_{\mu \in \mathrm{spec}(G)} j_\mu \tag{4}$$

of the *all-one vector* j in $\mathbb{R}^V$ into its components $j_\mu \in U_\mu$ relative to the canonical spectral decomposition

$$\mathbb{R}^V = \perp_{\mu \in \mathrm{spec}(G)} U_\mu$$

of $\mathbb{R}^V$ into the direct sum of the mutually orthogonal non-zero eigenspaces U_μ of A, and put

$$D_\mu := \langle j | j_\mu \rangle = \langle j_\mu | j_\mu \rangle$$

for every $\mu \in \mathrm{spec}(G)$. The eigenvalues μ with $D_\mu \neq 0$ are called the *main eigenvalues* of G and the quantities D_μ are called the (corresponding) main angles of G (cf [23]).

From

$$W_k = \sum_{v,w \in V} a_{vw}^{(k)} = j^{\mathrm{T}} A^k j \quad \text{and} \quad j = \sum_{\mu \in \mathrm{spec}(G)} j_\mu,$$

we get

$$W_k = \sum_{\mu \in \mathrm{spec}(G)} j^{\mathrm{T}} A^k j_\mu = \sum_{\mu \in \mathrm{spec}(G)} j^{\mathrm{T}} \mu^k j_\mu = \sum_{\mu \in \mathrm{spec}(G)} D_\mu \mu^k. \tag{5}$$

This is a well known result from spectral graph theory [22] (for an early chemical application, see [24]; other chemical applications are reported in [17, 20]).

Combining Eqs. (3) and (5), one obtains

$$\Delta_k = \sum_{\mu,\mu' \in \mathrm{spec}(G),\ \mu < \mu'} D_\mu \ D_{\mu'} \ (\mu \mu')^{k-1} \ (\mu - \mu')^2 . \tag{6}$$

Furthermore, the summation on the right–hand side of (6) may be restricted in case $k > 1$ to the non-zero main eigenvalues, only.

By means of Eq. (6), it is not difficult to show that [25, 26]

- $\Delta_{2k-1} \geq 0$ holds for all $k = 1, 2, \ldots$,
- one has $\Delta_1 = 0$ if and only if G is a regular graph if and only if $\Delta_k = 0$ holds for all $k = 1, 2, \ldots$.

It is less easy to determine the sign of Δ_k for even values of k. Examples show that this sign can attain any value, depending on both the structure of the graph G and the actual value of k.

In [26], the following result, shedding some light on the sign of Δ_k, was deduced from Eq. 6:

Theorem 1 *Given a finite graph G, exactly one of the following four alternatives holds:*

(H) $\Delta_1(G) \geq 0$ *and* $\Delta_k(G) = 0$ *for all* $k = 2, 3, \dots$,

(H₊) $\Delta_{2k-1}(G) > 0$ *for all and* $\Delta_{2k}(G) > 0$ *for all sufficiently large* k,

(H_-) $\Delta_{2k-1}(G) > 0$ *for all and* $\Delta_{2k}(G) < 0$ *for all sufficiently large* k,

(H_0) $\Delta_{2k-1}(G) > 0$ *and* $\Delta_{2k}(G) = 0$ *for all* $k = 1, 2, \dots$.

Graphs that satisfy (H) are said to be *harmonic*, and graphs that satisfy (H_+), (H_-), or (H_0) are called *super-*, *sub-*, and *almost harmonic*, respectively. Graphs with $\Delta_{2k}(G) > 0$ for all $k > 0$ are called *strictly* super- and those with $\Delta_{2k}(G) < 0$ for all $k > 0$ are said to be *strictly* subharmonic. We know that non-regular harmonic graphs exist as well as (strictly and not strictly) superharmonic and (strictly and not strictly) subharmonic graphs. Yet, we have not yet encountered any finite almost harmonic graph, and we strongly expect that no such graphs exist at all.

It is obvious from Eq. 6 that whether a graph is harmonic or sub-, super-, or almost harmonic can be deduced from its main eigenvalues and angles as follows (see also [26]):

Theorem 2 *Let G be a finite graph with exactly $N = N_G$ distinct main eigenvalues $\tau_1 = \tau_1(G) > \tau_2 = \tau_2(G) > \cdots > \tau_N = \tau_N(G)$ and corresponding main angles $D_{(i)} := D_{\tau_i}$. Then the following holds:*

(a) *G is regular in case $N = 1$ (as explained above).*

(b) *G is harmonic in case $N = 2$ and $\tau_N = 0$.*

(c) *G is strictly superharmonic in case $N \geq 2$ and $\tau_N > 0$.*

(d) *G is superharmonic in case $N \geq 2$ and $\tau_2 + \tau_N > 0$.*

(e) *G is subharmonic in case $\tau_2 + \tau_N < 0$.*

(f) *If $N \geq 2$ and $\tau_2 + \tau_N = 0$, then G is superharmonic in case $D_{(2)}(\tau_1 - \tau_2)^2 > D_{(N)}(\tau_1 + \tau_2)^2$, and G is subharmonic in case $D_{(2)}(\tau_1 - \tau_2)^2 < D_{(N)}(\tau_1 + \tau_2)^2$.*

(g) *If $N \geq 2$, $\tau_2 + \tau_N = 0$, and $D_{(2)}(\tau_1 - \tau_2)^2 = D_{(N)}(\tau_1 + \tau_2)^2$, then an additional (somewhat more complicated) examination is needed to determine to which class the graph G belongs.*

Remark 1 *If the graph G in the above theorem were almost harmonic, it would have to satisfy Condition (g), i.e. we would necessarily have $N = N_G \geq 2$, $\tau_2(G)+\tau_N(G) = 0$, and $D_{(2)}(\tau_1(G)-\tau_2(G))^2 = D_{(N)}(\tau_1(G)+\tau_2(G))^2$. Yet, while we encountered finite graphs G that satisfy Condition (g), none of those were almost harmonic.*

Remark 2 *Note that the Perron-Frobenius Theorem implies that*

$$\mu_G := \max(\mathrm{spec}(G))$$

coincides with $\max(|\mu| : \mu \in \mathrm{spec}(G))$ and that $D_{\mu_G} > 0$ always holds. Hence, $\mu_G = \tau_1(G) = \max(|\tau_1(G)|, |\tau_2(G)|, \ldots, |\tau_N(G)|) = \max(\tau_1(G), |\tau_N(G)|) > 0$ holds for every graph G with $E_G \neq \emptyset$.

Note also that the above considerations combined with the fact that there are exactly $d(v)^k$ walks $v_0, v_1, \ldots, v_{2k}$ in G with $v_0 = v_2 = \cdots = v_{2k}$ for each vertex $v \in V$ implies — even without the use of the Perron-Frobenius Theorem — that

$$\max(|\tau_1(G)|, |\tau_2(G)|, \ldots, |\tau_N(G)|) = \max(\tau_1(G), |\tau_N(G)|) \geq \sqrt{\max(d(v) : v \in V)}$$

always holds and that $D_{(1)} \geq D_{(N)}$ holds in case $\tau_N(G) = -\tau_1(G)$ (while the well-known result (cf. [22]) that there is some bipartite connected component G' with $\mu_G = \mu_{G'}$ in this case even implies that $D_{(1)} > D_{(N)}$ must hold in case $\tau_N(G) = -\tau_1(G)$).

Remark 3 *All harmonic trees (including the infinite harmonic trees) were recently determined in [27] where it was shown in particular that a finite tree T with at least 3 vertices is harmonic if and only if it has exactly one vertex v of degree $a^2 - a + 1$ for some integer $a = a(T) \geq 2$ while all neighbours of v have degree a and all other vertices are leaves. Thus, a finite harmonic tree with at least 3 vertices has*

$$a^3 - a^2 + a + 1 = 7,\ 22,\ 53,\ \text{or}\ \ldots$$

vertices. In addition, also all harmonic graphs with a small number of cycles were recently determined (cf. [28]): There are 0, 0, 4, and 18 connected non-regular unicyclic, bicyclic, tricyclic, and tetracyclic harmonic graphs, respectively. In contrast, not a single example of an almost harmonic graph has been found so far, and we conjecture that such graphs do not exist at all.

Remark 4 *It follows from Theorem 2 (e) that every finite connected bipartite graph $G = (V, E)$ with bipartition $V = V_1 \cup V_2$ is subharmonic provided one has $\sum_{v \in V_1} a_v \neq \sum_{v \in V_2} a_v$ for one and, hence, for every positive eigenvector $(a_v)_{v \in V}$ as this implies $\tau_N(G) = -\tau_1(G)$ and hence $\tau_2(G) + \tau_N(G) = -(\tau_1(G) - \tau_2(G)) < 0$.*
Thus, unless $\sum_{v \in V_1} a_v = \sum_{v \in V_2} a_v$ holds in view of the existence of a "switching symmetry" of G, i.e. an automorphism that interchanges V_1 and V_2 (in which case a "switching involution", i.e. a switching symmetry of order 2, must exist[1]), a "generic" finite and connected bipartite graph should be expected to be subharmonic.

The least and the most branched n-vertex trees (the path and the star) were shown in [26] to be strictly subharmonic for all $n \geq 3$, and this finding — together with the fact mentioned above that any finite bipartite graph G has always a good chance of being subharmonic — pointed towards the possibility that all trees, being surely bipartite, might be either harmonic or (perhaps even strictly) subharmonic.

In order to collect more empirical data on the behaviour of (the sign of) Δ_k, we have studied systematically all 205,004 trees with up to 18 vertices by means of computer-aided calculations, and we will discuss some basic computational aspects of this work in the subsequent sections and the appendix.

Our results can be summarized as follows: Among all those 205,004 trees with up to 18 vertices, Case (a) ($N_G = 1$) occurs (obviously) for the two trees with at most two vertices, only. In accordance with [27], Case (b) occurs only for the unique harmonic 7-vertex tree T with $a(T) = 2$. Among the remaining 205,001 trees with up to 18 vertices, 204,431 (and, thus, more than 99,7% of those) are subharmonic for "trivial" reasons because their smallest eigenvalue is a main eigenvalue while 486 trees of the remaining 570 trees with $-\tau_1(G) \neq \tau_N(G)$ have a switching symmetry. Yet, only 2 of those 486 are superharmonic (both having 18 vertices), and only 9 of the remaining 84 trees are superharmonic (i.e. among those 84 non-harmonic trees with up to 18 vertices that do not have a switching symmetry inspite of the fact that their smallest eigenvalue is not a main eigenvalue). None of the 2 superharmonic trees with a switching symmetry and exactly one of the other 9 superharmonic trees is strictly superharmonic (the tree T_4 in Figure 2). Thus, altogether only 11 of the

[1] Indeed, if φ is a switching symmetry of order $2^a(2b-1)$ for some positive integers a, b, the power $\psi := \varphi^{2b-1}$ is a switching symmetry of order 2^a and must therefore fix some edge $\{u, v\} \in E$ in view of $\#E = \#V - 1 = \#V_1 + \#V_2 - 1 = \#V_1 + \#V_1 - 1 \equiv 1 \mod 2$ implying that the map $\psi' : V \to V$ that coincides with ψ on all vertices w that are closer to, say, u than to v and with ψ^{-1} on the remainnig vertices of V is a switching automorphism of G of order 2.

205,004 trees with up to 18 vertices are superharmonic of which exactly one is actually strictly superharmonic. In particular, even though we now do know that there are finite superharmonic trees, such trees are evidently quite rare even among those trees G with $-\tau_1(G) \neq \tau_N(G)$, and not even the existence of a switching symmetry appears to increase the likelihood of being superharmonic.

Moreover, while we never observed a tree G with $N = N_G \geq 2$ and $\tau_N(G) > 0$ (Case (c) in Theorem 2) or with $N = N_G \geq 2$, $\tau_2(G) + \tau_N(G) = 0$, and

$$D_{(2)}\,(\tau_1(G) - \tau_2(G))^2 = D_{(N)}\,(\tau_1(G) + \tau_2(G))^2$$

(Case (g) in Theorem 2), examples for every other of the seven cases considered in that theorem were encountered.

2 The Naive Direct Approach

Using Eqs. (2) and (3), the W_k- and Δ_k-values, $k = 1, 2, \ldots$, are readily computed from the adjacency matrix of a given graph. For this, a computer program was employed written in FORTRAN 77. When we started our research, we hoped that the *asymptotic* behaviour of the sequence $(\Delta_k)_{k\in\mathbb{N}}$ as described in Theorem 1 would show up *early* enough so that we could infer the sub– or superharmonicity of a small graph on the basis of the signs of those Δ_k-values that we could still handle by this FORTRAN program[2]. In other words, we hoped that — at least for any tree with up to 18 vertices — the sign of Δ_{2k} would not change any more above those values of k that could be accessed by computer in the way described above: If $\Delta_{2k} < 0$ would hold for any such "sufficiently large" value of k, the respective graph G could be recognized as subharmonic while $\Delta_{2k} > 0$ would imply that G is superharmonic. This will be referred to as the "direct approach".

Yet, the exponential growth of W_k causes the following technical limitation: For every graph, there is a maximal value of k beyond which an overflow occurs and the calculation is interrupted. In the present case, the maximal accessible value of k was usually around 20. For instance, it was between 18 and 30 for trees with 8 vertices

[2]This hope could have been based in particular on the fact that the actual values of the first $2N$ numbers $W_0, W_1, \ldots, W_{2N-1}$ determine the set $\{\tau_1, \tau_2, \ldots, \tau_N\}$ as well as the corresponding angles $D_{(1)}, D_{(2)}, \ldots, D_{(N)}$ uniquely and that the number N of main eigenvalues can also be deduced from the sequence $(W_k)_{k=0,\ldots,\#V}$ as it coincides with the rank of the associated *Hankel matrix* $(W_{i+j})_{i,j=0,\ldots,N}$, see the appendix for details.

and between 13 and 27 for trees with up to 18 vertices.

k	$W_k(T_A)$	$\Delta_k(T_A)$	$W_k(T_B)$	$\Delta_k(T_B)$
1	22	68	22	68
2	46	−48	46	−180
3	94	272	88	628
4	198	−100	182	−2148
5	416	1580	352	7864
6	882	828	724	−28560
7	1872	11268	1408	107000
8	3986	16316	2886	−396324
9	8496	92136	5634	1493220
10	18132	195696	11516	−5571556
11	38720	821960	22550	21003180
12	82730	2062620	45980	−78617000
13	176816	7711224	90268	296191056
14	377996	20654288	183656	−1110462392
15	808194	74389572	361358	4180924332
16	1728198	201717192	733766	−15689405140
17	3695734	729472220	1446552	59040379092
18	7903712	1939763080	2932206	−221682608388
19	16903436	7235260656	5790424	833899065416
20	36151796	18410103392	11719132	−3132239700624
21	77319828	72486857776	23177200	11779489589416
22	165370160	172157862776	46843238	−44255941970244
23	353692742	734002490236	92765002	166405791184036
24	756480430	1577920106708	187257580	−625290185902596
25	–	–	371261902	2350868472612716
26	–	–	748628004	−8834589729432696

Table 1. *W_k and Δ_k for two 12-vertex chemical trees: the molecular graph T_A of 5,6-dimethyldecane, and the molecular graph T_B of 2,9-dimethyldecane (cf. Figure 1). Note that T_A appears to be superharmonic whereas T_B appears to be strictly subharmonic. However, while the latter conclusion can be shown to be indeed correct, the former is not (see text and Table 2) implying that the naive "direct approach" is insufficient for gaining reliable insights about the sub- and superharmonicity of trees.*

Results of two typical calculations are shown in Table 1. We computed W_k and Δ_k for all trees up to 20 vertices until overflow occured. In full agreement with Theorem 1, we found that, except for the three harmonic trees with 1, 2, and 7 vertices, Δ_k is positive for all of these trees for all odd $k \in \mathbb{N}$. However, a detailed examination revealed that our "direct approach" is not sufficient to establish that a tree is sub- or superharmonic: The values $\Delta_k(T_A)$ of the tree T_A continuously increase for even k from -100 for $k := 4$ to $1,577,920,106,708$ for $k := 24$, suggesting that the tree T_A

should be superharmonic. In this case however, the ratios Δ_k/Δ_{k-2} (k even) should be approaching their limit from below (which limit then also had to be the square of the largest number λ of the form $\lambda = \mu\,\mu'$ with $\mu, \mu' \in \mathrm{spec}(G)$ and $a_\lambda \neq a_{-\lambda}$ where a_λ is defined by $a_\lambda := \sum_{\mu,\mu' \in \mathrm{spec}(G),\, \lambda=\mu\mu'} D_\mu \ D_{\mu'} \ (\mu - \mu')^2)$ while the data given in Table 1 imply that the sequence Δ_k/Δ_{k-2} is monotonously decreasing for even k from $k := 8$ to $k := 24$. This indicates clearly that the long-term behaviour of the $\Delta_k(T_A)$-values and their signs cannot safely be deduced for even k from the values and signs of the first 12 values $\Delta_2(T_A), \Delta_4(T_A), \ldots, \Delta_{24}(T_A)$ given in Table 1.

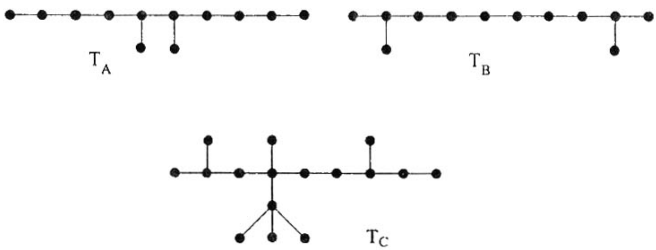

Figure 1. *The trees T_A, T_B, and T_C*

And indeed, as can be shown by the methods explained below, $\tau_2 + \tau_N < 0$ holds for T_A (i.e. Case (e) applies to T_A) and the Δ_k-values of the tree T_A computed using an appropriate version of *MAPLE* for all even integers k up to $k := 48$ are all negative from $k := 36$ on (cf. Table 2) and can be proven to remain negative for all larger even integers k as well. This fact can, of course, not at all be guessed from just glancing at the data found in Table 1 (though, as mentioned above and shown in the appendix, it could have been deduced from these data by much more elaborate computations). The reason for such an "irregular" behavior of the first 20–30 $\Delta_k(T_A)$ values is the very small size of $D_{(N)}$ relative to $D_{(2)}$. Namely, for the tree T_A we have $\tau_2 = 1.45989$, $D_{(2)} = 2.00019$ and $\tau_N = -1.70504$, $D_{(N)} = 0.00036$.

However, even the pattern of signs in Table 2 is in no way sufficient to firmly conclude that the tree T_A is subharmonic. They only imply that T_A is neither strictly subharmonic nor strictly superharmonic. In order to deduce from such a table more or less reliably whether a tree with, say, up to 20 vertices is sub- or superharmonic, it is probably necessary to compute its Δ_k-values for k well beyond 100. And even then, without additional evidence, we could not be completely certain that our conclusions would be correct.

k	$W_k(T_A)$	$\Delta_k(T_A)$
25	1617969924	7525503334384
26	3460544512	14032966377128
27	7401486378	78310807410972
28	15830479488	118782938373516
29	33858631470	829330443913404
30	72417753058	917966468333276
31	154889068112	8961723340508788
32	331281092954	5755015235157116
33	708553351386	99026831640465224
34	1515474204430	13614337520753744
35	3241339658354	1120464125966189244
36	6932670889792	−432443355915485476
37	14827796621022	12985357245959838076
38	31714121312680	−11732702471263166068
39	67831081354106	154015119131905565724
40	145079086578472	−214353735226099655328
41	310299360232976	1866152511517240178368
42	663677288697752	−3419309680469574618272
43	1419492259936282	23042614116042618807612
44	3036051305922068	−51017389785142741138416
45	6493594746044944	289134849820233520918296
46	13888689210471374	−732533926091051831381732
47	29705532112242926	3676451248194800524753184
48	63535055639566590	−10268993009027211743444116
49	135890623658955784	47247877667850844273976504

Table 2. *W_k and Δ_k for the molecular graph T_A of 5, 6-dimethyldecane for larger values of k (cf. Table 1). These data are sufficient to claim that T_A is not strictly superharmonic, but not to decide whether it is sub- or superharmonic.*

In Table 3, we illustrate yet another weak point of the "direct approach". In the case of the tree T_C — the molecular graph of 2, 4, 7-trimethyl-4-*tert*-butylnonane ($n = 16$), $\Delta_k(T_C)$ is negative for even numbers k up to $k = 36$, hinting towards the possibility that T_C is strictly subharmonic. Then, for $38 \leq k \leq 54$, the Δ_k-values are positive, suggesting superharmonicity. Only when k exceeds 54, Δ_k becomes negative again for even k and probably remains negative for all even $k \geq 56$. This example shows that, even though strictness can definitely be *disproved* by computing the signs of sufficiently many Δ_k-values, the naive direct approach cannot be used that easily for *proving* that a tree is strictly sub- or superharmonic.

In summary: The naive direct approach was found to be unable to serve its purpose and had to be abandoned, and other, computationally more demanding and, from

$2k$	$\Delta_{2k}(T_C)$
2	−616
4	−7864
6	−119556
8	−1936560
10	−32143020
12	−538676948
14	−9053235488
16	−151980856232
18	−2540974364448
20	−42192557158844
22	−693638472648884
24	−11243975183533360
26	−178668845293823716
28	−2757598667159179516
30	−40690162183065801484
32	−556386768219784654320
34	−6529496017196673730904
36	−48271348722870087779556
38	507003868815924255443424
40	36289514317018021740231980
42	1180926160001921976793959740
44	31165486754137308102443252720
46	734144499880100262063341269120
48	15756939423401815255741381765240
50	301714217416097306852302865378204
52	4654169274049470568618646581368116
54	29276576319690047698978623364719176
56	−1883120203759299863282577365860763196
58	−126526291994352059350645136900779826236
60	−5618728087243412090304580558749272389084
62	−217699239480595001153697197265350964643704
64	−7908469386021268897703975161363101580966728
66	−277395384686898311330933876848472398634947108
68	−9532607914649309506765937115284611891191771872
70	−323537515741240552653520209472570806695522691724
72	−108964844479986146759657466623812040423389487682388
74	−365209089625273972114894119074197359284933909539776
76	−12202890874513453232014763107691161236954755080746056
78	−406944856873717750596569702188233742431711819514157824
80	−13554008022795091545532739474455550971853221680058498252

Table 3. Δ_{2k}*-values for the molecular graph* T_C *of 2,4,7-trimethyl-4-tert-butylnonane. This example illustrates the difficulties in establishing strictly sub- and superharmonicity. Analysis based on Theorem 3 shows that* T_C *is subharmonic.*

a numerical point of view, much more elaborate methods of calculation based on Theorem 2 had to be pursued.

3 Other Methods of Computation

To determine whether a given tree is sub– or superharmonic, one can of course make use of Theorem 2. However, a direct application of that theorem is not that easy. The main problem is determining which graph eigenvalues are main and which are not, because the apparently very simple criterion "$D_\mu > 0$ for main and $D_\mu = 0$ for non-main eigenvalues" is not always easy to apply in practice. Indeed, we have encountered some non-zero D_μ-values below 0.0000001 that are clearly difficult to distinguish from 0 in standard numerical computations.

We have overcome these difficulties by applying suitable results from spectral graph theory. Our first method makes use of the *complement*

$$\overline{G} := \left(V_G, \binom{V_G}{2} - E_G \right)$$

of a graph $G = (V, E)$, i.e. that graph $\overline{G}$ whose adjacency matrix $A_{\overline{G}}$ coincides with the matrix $J - (I + A_G)$ where J is the *all-one matrix* and I is the unit matrix. By reference to this graph, the main eigenvalues of G can be characterized as follows:

Theorem 3 [22, p. 55] *A real number μ is a main eigenvalue of a graph G if and only if*

$$\dim U_\mu(G) = \dim U_{-\mu-1}(\overline{G}) + 1$$

holds. In particular, if $\dim U_\mu(G) = 1$ holds, then μ is a main eigenvalue if and only if $-\mu - 1$ is not an eigenvalue of $\overline{G}$.

Another method for determining all main eigenvalues of a graph G can be based on the following observation that will also be detailed in the appendix

Theorem 4 *Let $j \in \mathbb{R}^V$ be the all-one vector and consider the vectors $A^i j \in \mathbb{R}^V$ ($i \in \mathbb{N}_0$). Let M be the smallest number such that the vectors $j, Aj, \ldots, A^M j$ are linearly dependent. Then M coincides with the number $N = N_G$ of distinct main eigenvalues of G, there exist unique integers $z_0, z_1, \ldots, z_{N-1}$ with*

$$A^N j = z_0 j + z_1 Aj + \cdots + z_{N-1} A^{N-1} j,$$

and the main eigenvalues of G are exactly the roots of the polynomial

$$main_G(x) := x^N - z_{N-1}\, x^{N-1} - z_{N-2}\, x^{N-2} - \cdots - z_0.$$

In particular, this polynomial has simple roots, only.

Remark 5 *Note that for obtaining the polynomial $main_G(x)$, only integer calculations are needed. Note also that its coefficients $z_0, z_1, \ldots, z_{M-1}$ provide a recursive formula for the vectors $A^i_G j$ and the number of walks of length $k \geq M$: Indeed, we have*

$$W_k = \sum_{i=1}^{M} z_{M-i} W_{k-i}$$

for all $k \geq M$.

By means of either of the above two results, it is possible to determine the main eigenvalues of a graph by computing eigenvalues only, i.e. without computing the eigenvectors. In our calculations, we first employed Theorem 3 in the following way: For any tree T from our list with n vertices, we computed the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n$ of T and the eigenvalues $\overline{\lambda}_1 \geq \overline{\lambda}_2 \geq \cdots \overline{\lambda}_n$ of its complement $\overline{T}$ (with multiplicities) up to 12 decimal places, and considered equality to hold between an eigenvalue λ_i of G and a term of the form $-1-\overline{\lambda}_j$ for some eigenvalue $\overline{\lambda}_j$ of $\overline{T}$ if the difference $\lambda_i + \overline{\lambda}_j + 1$ was smaller than $5 \cdot 10^{-10}$.

In a second step, we also calculated the main eigenvalues of all trees in our list using Theorem 4 (the *MAPLE* subroutine developed for this task is available at `www.mathematik.uni-bielefeld.de/~grunew/mvalues`).

Once the main eigenvalues of a graph are known, its sub- or superharmonicity can easily be decided in the Cases (b), (c), (d), and (e) (see Theorem 2). Only in Case (f), it is necessary to compute $D_{(2)}$ and $D_{(N)}$. Yet, these values never needed to be computed with a very high accuracy to reach a conclusion. Luckily, the Case (g) has never been encountered among the trees examined (nor was any tree with 18 or fewer vertices found to be almost harmonic, nor did the Case (c) ever occur). Applying this kind of reasoning to the results of both computations, exactly the same trees were found to be sub- or superharmonic, respectively, thus corroborating our findings beyond reasonable doubt.

Two typical results are presented in Table 4. These pertain to the superharmonic trees T_2 and T_5 depicted in Figure 2.

Remark 6 *Note that we could also have used Theorem 3 to determine the polynomial $main_G(x)$ by integer calculations only: Indeed, denoting the derivative $na_n x^{n-1} + (n-1)a_{n-1}x^{n-2} + \cdots + a_1$ of a polynomial $p(x) := a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$ by $p'(x)$ as usual and defining polynomials $p_1(x)$ to $p_9(x)$ as follows*

$$p_1(x) := det(xI - A_G),$$

$$p_2(x) := gcd(p_1(x), p_1'(x)),$$

$$p_3(x) := det(xI - A_{\overline{G}}) = det(xI - J + I + A_G),$$

$$p_4(x) := (-1)^{\#V} p_3(-1-x) = det(J + xI - A_G),$$

$$p_5(x) := gcd(p_2(x), p_4(x)),$$

$$p_6(x) := p_2(x)/p_5(x),$$

$$p_7(x) := p_4(x)/p_5(x),$$

$$p_8(x) := gcd(p_1(x)/p_2(x), p_6(x)p_7(x)),$$

$$p_9(x) := p_1(x)/(p_2(x)p_8(x)),$$

it follows immediately from Theorem 3 that, up to normalization if required, $main_G(x) = p_9(x)$ *must hold.*
Alternatively, one can also compute $main_G(x)$ *usind the following sequence of polynomials:*

$$q_1(x) := p_1(x) = det(xI - A_G),$$

$$q_2(x) := p_4(x) = det(J + xI - A_G),$$

$$q_3(x) := gcd(q_1(x), q_2(x)),$$

$$q_4(x) := q_1(x)/q_3(x),$$

$$q_5(x) := q_4',$$

$$q_6(x) := gcd(q_4(x), q_5(x)^2),$$

$$q_7(x) := q_4(x)/q_6(x).$$

Then, also $main_G(x) = q_7(x)$ *must hold.*
However, we did not run either of these two routines for computing $main_G(x)$ *because we considered the evidence derived from the fact that the two procedures desribed further above yielded the same result to be sufficiently convincing.*

4 Discussion

By means of the calculation techniques described in the previous section, we have examined all trees with $n \leq 18$ vertices in two independent ways and established for any such tree whether it is harmonic, almost harmonic, superharmonic or subharmonic. For reasons explained above (cf. Table 3), we did not endeavor to distinguish between strictly and non-strictly subharmonic trees.

Our main findings are the following

- Among trees with 18 or fewer vertices, there is no one that is almost harmonic.
- Most trees with 18 or fewer vertices, altogether such 204,990 trees, are subharmonic. For 204,431 of them, the smallest eigenvalue is a main eigenvalue.
- There exist exactly 11 superharmonic trees with 18 or fewer vertices, viz. the trees T_1 to T_{11} in Figure 2. The smallest of those has 12 vertices. The only strictly superharmonic tree with at most 18 vertices is the tree T_4.

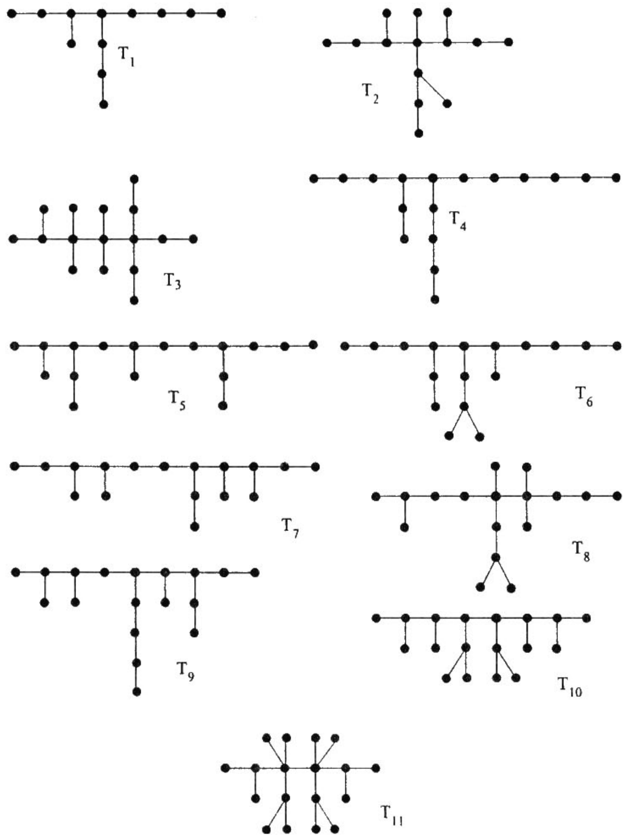

Figure 2. *The* 11 *superharmonic trees with* 18 *or fewer vertices. The smallest superharmonic tree T_1 has* 12 *vertices and is characterized by that property among all trees with at most that many vertices. Note that only the last one of those 11 trees is not a "chemical" tree because it has vertices of degree above* 4.

The following problems, however, remain open:

- Are there any trees (or, at least, graphs) that are almost harmonic?

- As mentioned already above, it has been shown in [25] that, for any finite graph G, there exists a unique smallest number $k(G)$ such that

$$\mathrm{sign}(\Delta_{2k(G)}(G)) = \mathrm{sign}(\Delta_{2k}(G))$$

  holds for all $k \geq k(G)$. Thus, as there are only finitely many graphs with up to n vertices, there exists a unique smallest even number $k(n)$ for any number n such that any tree T with up to n vertices and $\Delta_{k(n)}(T) > 0$ is superharmonic, and any tree T with up to n vertices and $\Delta_{k(n)}(T) < 0$ is subharmonic, viz. the maximum of the numbers $k(T)$ over all trees T with up to n vertices.

  Thus, if an upper bound for the number $k(n)$ could be computed without first computing the numbers $k(T)$ for all trees T with up to n vertices, the naive "direct approach" would work indeed for the trees studied in this paper provided we could compute the numbers $\Delta_{k(18)}(T)$ for all trees T with up to 18 vertices. Since $\Delta_{160} < 0$ holds for the superharmonic tree T_6 with 17 vertices, $k(18)$ must be at least 162.

  However, we do not know how to derive such an upper bound by direct reasoning, we have no idea whether the function $k(n)$ can be expected to grow linearly or, at least, polynomially with n, nor do we expect the number $k(n)$ to be small enough so that computing those numbers $\Delta_{k(n)}$ in the naive fashion described in Section 2 would be feasible.

- Is the fact that less than 2% of the trees with 18 or fewer vertices whose smallest eigenvalue is not a main eigenvalue are superharmonic a "small number phenomenon"? More precisely: What can be said about the ratio of the number of sub- and superharmonic trees with n vertices whose smallest eigenvalue is not a main eigenvalue for n going to infinity?

- Finally, it would also be of interest to know whether the ratio of the number of trees with n vertices whose smallest eigenvalue is a main eigenvalue and the number of all trees with n vertices goes to 1 for n going to infinity?

The computational details by means of which it could be established that T_2 and T_5 are superharmonic are found in the caption of Table 4. Case (d) of Theorem 2 is applicable for the trees T_1, T_2, T_3, T_4, T_6, T_8, T_9, T_{10}, and T_{11}. Case (f) of Theorem 2 is applicable to the trees T_5 and T_7. As a curiosity, we mention that for this latter tree, $D_{(2)}\,(\tau_1 - \tau_2)^2 = 0.026245$ is only slightly, but clearly enough above $D_{(N)}\,(\tau_1 + \tau_2)^2 = 0.025585$.

i		$\lambda_i(T_2)$	$D_{(i)}(T_2)$	$-1-\lambda_{15-i}(\bar{T}_2)$
1	M	2.414213562373	10.24264	1.618033988750
2		1.618033988750	.00000	1.618033988750
3		1.618033988750	.00000	1.284434588588
4	M	1.000000000000	2.00000	.618033988750
5		.618033988750	.00000	.618033988750
6		.618033988750	.00000	.414213562373
7		.414213562373	.00000	−.063707558882
8	M	−.414213562373	1.75736	−.618033988750
9		−.618033988750	.00000	−.618033988750
10		−.618033988750	.00000	−1.000000000000
11		−1.000000000000	.00000	−1.618033988750
12		−1.618033988750	.00000	−1.618033988750
13		−1.618033988750	.00000	−2.414213562373
14		−2.414213562373	.00000	−12.220727029706

i		$\lambda_i(T_5)$	$D_{(i)}(T_5)$	$-1-\lambda_{18-i}(\bar{T}_5)$
1	M	2.193527085331	13.05251	2.046970621622
2	M	2.035648404257	.96169	1.712215502960
3	M	1.690692744042	.58352	1.305732112092
4	M	1.294962899292	.15219	1.193527085331
5		1.193527085331	.00000	.899670904634
6	M	.884132539245	.10981	.643891143493
7	M	.464761522222	1.62404	.294962899292
8		.294962899292	.00000	.000000000000
9		.000000000000	.00000	−.294863164756
10	M	−.294962899292	.00064	−.456262907790
11	M	−.464761522222	.04939	−.844838401178
12	M	−.884132539245	.19413	−1.180658883726
13	M	−1.193527085331	.06156	−1.294962899292
14		−1.294962899292	.00000	−1.639951477270
15	M	−1.690692744042	.21035	−2.035609187735
16	M	−2.035648404257	.00016	−2.193527085331
17		−2.193527085331	.00000	−15.156296262346

Table 4. *Numerical data needed for applying Theorem 3. M indicates the main eigenvalues. The tree T_2 is superharmonic because $\tau_2 = 1.00000$ is greater than $|\tau_N| = 0.414214$ (Case (d) in Theorem 2) while T_5 is superharmonic because $D_{(2)}\,(\tau_1 - \tau_2)^2 = 0.02397$ is greater than $D_{(N)}\,(\tau_1 + \tau_2)^2 = 0.00287$ (Case (f) in Theorem 2).*

5 Appendix

Let us note first that, given any field K and any map $\Phi : K \to K$ of finite support, one can always recover the map Φ from the first few terms of the associated sequence

$$\mathcal{W}(\Phi) := \left(\sum_{\tau \in K} \Phi(\tau)\tau^k\right)_{k \in \mathbb{N}_0}.$$

More precisely, denoting the k-th term $\sum_{\tau \in K} \Phi(\tau)\tau^k$ in that sequence for every $k \in \mathbb{N}_0$ by $W_k = W_k(\Phi)$, the following facts are well known from the theory of linearly recursive sequences:

Theorem 5 *The cardinality of the support* $\operatorname{supp}(\Phi) = \{\tau \in K : \Phi(\tau) \neq 0\}$ *of* Φ *coincides with the smallest integer* $N \in \mathbb{N}_0$ *for which the determinant of the associated* $(N+1) \times (N+1)$ *Hankel matrix*

$$\mathbf{H}(\mathcal{W}(\Phi), N) = (W_{i+j})_{i,j=0,\ldots,N}$$

vanishes, the support of Φ *consists of the (necessarily distinct) zeros of the polynomial*

$$x^N - z_{N-1}x^{N-1} - z_{N-2}x^{N-2} - \cdots - z_0$$

where the coefficients $z_0, z_1, \ldots, z_{N-1}$ *are the (necessarily unique) elements in* K *with*

$$W_{i+N} = z_0 W_i + z_1 W_{i+1} + \cdots + z_{N-1} W_{i+N-1} \tag{7}$$

for all $i = 0, \ldots, N-1$, *while — given the number* N *and the set* $\operatorname{supp}(\Phi)$ *— the images* $\Phi(\tau)$ *of the elements* $\tau \in \operatorname{supp}(\Phi)$ *are, essentially by definition, solutions of the system of* N *linear equations*

$$W_i = \sum_{\tau \in \operatorname{supp}(\Phi)} \Phi(\tau)\tau^i \quad (i = 0, \ldots, N-1)$$

and thus are uniquely determined by the number N, *the set* $\operatorname{supp}(\Phi)$, *and the first* N *terms* $W_0, W_1, \ldots, W_{N-1}$ *of the sequence* $\mathcal{W}(\Phi)$ *in view of the fact that the determinant of the Vandermonde matrix*

$$\mathbf{V}(\operatorname{supp}(\Phi)) := (\tau^k)_{\tau \in \operatorname{supp}(\Phi), i=0,\ldots,N-1}$$

does not vanish.

Moreover, the recursion (7) *that allows to determine the terms* W_N, W_{N+1}, W_{2N-1} *of the sequence* $\mathcal{W}(\Phi)$ *from the first* N *terms* W_0, W_1, W_{N-1}, *holds for all* $i \in \mathbb{N}_0$ *and, thus, allows to compute all the terms* W_k *in that sequence from its first* N *term in a linearly recursive fashion (provided one knows already the coefficients* $z_0, z_1, \ldots, z_{N-1}$*).*

Proof: Indeed, labelling the N elements in $\operatorname{supp}(\Phi)$ by $\tau_1, \tau_2, \ldots, \tau_N$ and denoting

(i) the $(M+1) \times N$ matrix $(\tau_j^i)_{i=0,\ldots,M, j=1,\ldots,N}$ by $\mathbf{T}_M$,

(ii) the coefficients of the polynomial $p(x) := \prod_{i=1,\dots,N}(x - \tau_i)$ by $z_0, z_1, \dots, z_{N-1}$ so that

$$p(x) = \prod_{i=1,\dots,N} (x - \tau_i) = x^N - z_{N-1}\, x^{N-1} - z_{N-2}\, x^{N-2} - \dots - z_0$$

holds,

(iii) the Φ-image $\Phi(\tau_i)$ of τ_i by $D_{(i)}$ for $i = 1, \dots, N$,

(iv) and the non-singular diagonal $N \times N$ matrix $(\delta_{ij} D_{(i)})_{i,j=1,\dots,N}$ by $\mathbf{D}$,

it is easily seen that the identity

$$\mathbf{H}(\mathcal{W}(\Phi), M_1, M_2) = \mathbf{T}_{M_1} \mathbf{D}\, \mathbf{T}^t_{M_2}$$

holds for the Hankel matrices

$$\mathbf{H}(\mathcal{W}(\Phi), M_1, M_2) := (W_{i+j})_{i=0,\dots,M_1\, j=0,\dots,M_2}$$

for all $M_1, M_2 \in \mathbb{N}_0$, and that the product

$$(z_0, z_1, \dots, z_{N-1}, -1)\ \mathbf{T}_N$$

of the $(N+1)$ vector $(z_0, z_1, \dots, z_{N-1}, -1)$ with the $(N+1) \times N$ matrix $\mathbf{T}_N$ coincides with the N vector $(p(\tau_1), p(\tau_2), \dots, p(\tau_N))$ and, thus, vanishes. The assertions of the theorem follow immediately from these simple (and well-known) observations. ∎

The claim stated in the footnote in Section 2 follows immediately from Theorem 5. To establish also the claims made in Theorem 4, recall first that, given

(i) a field K,

(ii) a $n \times n$ matrix $A = (a_{ij})_{i,j=1,\dots,n}$ with coefficients $a_{ij} \in K$ and eigenspaces $U_\mu = U_\mu(A) := \{u \in K^n | Au = \mu u\}$ $(\mu \in K)$,

(iii) and a vector $j \in K^n$,

the dimension $N(A, j)$ of the subspace

$$U = U(A, j) := \langle A^k j \,:\, k \in \mathbb{N}_0 \rangle_K$$

of K^n spanned by the vectors in the A-invariant subset $\{j, A\,j, A^2\,j, A^3\,j, \dots\}$ of K^n generated by the vector j, always coincides with the smallest integer N for which the vector $A^N\,j$ can be expressed as a linear combination

$$A^N\,j = \sum_{k=0,\dots,N-1} z_k\, A^k\, j \tag{8}$$

of the preceding vectors $j, A\,j, A^2\,j, A^3\,j, \dots, A^{N-1}\,j$, and the polynomial

$$p_{A,j}(x) := x^N - z_{N-1}\, x^{N-1} - z_{N-2}\, x^{N-2} - \dots - z_0$$

defined in terms of the coefficients $z_0, z_1, \ldots, z_{N-1} \in K$ in that linear combination is the characteristic polynomial of the linear operator $A\big|_U : U \to U$ defined by restricting the linear operator A to the (A-invariant!) subspace $U = U(A, j)$.

Thus, if

$$\operatorname{spec}_K(A) := \{\mu \in K \,:\, \dim U_\mu > 0\}$$

denotes the set of eigenvalues of A in K, if

$$j \in \bigoplus_{\mu \in \operatorname{spec}_K(A)} U_\mu$$

holds (in particular, if $K^n = \oplus_{\mu \in \operatorname{spec}_K(A)} U_\mu$ holds, i.e. if A is diagonalizable and K contains all eigenvalues of A), and if

$$j = \sum_{\mu \in \operatorname{spec}_K(A)} j_\mu \tag{9}$$

is the corresponding decomposition of the vector j into its components $j_\mu \in U_\mu$, the number $N(A, j)$ coincides also with the cardinality $s := \#\operatorname{spec}_K(A, j)$ of the set

$$\operatorname{spec}_K(A, j) := \{\mu \in \operatorname{spec}_K(A) \,:\, j_\mu \neq 0\}$$

because we have clearly

$$U(A, j) \subseteq \langle j_\mu \,:\, \mu \in \operatorname{spec}_K(A)\rangle_K = \langle j_\mu \,:\, \mu \in \operatorname{spec}_K(A, j)\rangle_K \tag{10}$$

in view of

$$A^k j = \sum_{\mu \in \operatorname{spec}_K(A,j)} \mu^k j_\mu \in \langle j_\mu \,:\, \mu \in \operatorname{spec}_K(A, j)\rangle_K$$

for all $k \in \mathbb{N}_0$ while the non-vanishing of the determinant of the Vandermonde matrix

$$\mathbf{V}(\operatorname{spec}_K(A, j)) := (\mu^k)\mu \in \operatorname{spec}_K(A, j), k = 0, \ldots, s-1$$

implies that the elements

$$A^k j = \sum_{\mu \in \operatorname{spec}_K(A,j)} \mu^k j_\mu \quad (k = 0. \ldots, s-1)$$

actually form a basis of the space $\langle j_\mu \,:\, \mu \in \operatorname{spec}_K(A, j)\rangle_K$ yielding that equality must hold in (10), that

$$U(A, j) = \bigoplus_{\mu \in \operatorname{spec}_K(A,j)} \langle j_\mu \rangle_K$$

is the eigenspace decomposition of $U(A, j)$ relative to the linear operator $A\big|_U$ that maps U into itself, and that the polynomial

$$p_{A,j}(x) = x^N - z_{N-1}\, x^{N-1} - z_{N-2}\, x^{N-2} - \cdots - z_0$$

considered above must therefore coincide with the product $\prod_{\mu \in \operatorname{spec}_K(A,j)}(x - \mu)$.

This implies all assertions of Theorem 4 except the assertion that the coefficients $z_{N-1}, \cdots, z_0$ must be integers in the specific case considered in that theorem. However, this is a simple consequence of the fact that in case K is the real number field $\mathbb{R}$, and A and j have integer coefficients, the coefficients $z_{N-1}, \cdots, z_0$ satisfying the identity (8) must be rational numbers on the one hand and algebraic integers on the other because the roots of the polynomial $p_{A,j}(x) = x^N - z_{N-1}x^{N-1} - z_{N-2}x^{N-2} - \cdots - z_0$, being also roots of the characteristic polynomial of A, are necessarily algebraic integers. This, finally, establishes Theorem 4.

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