THE MATCHING ENERGY OF A GRAPH

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ABSTRACT. The energy of a graph G is equal to the sum of the absolute values of the eigenvalues of G. We define the matching energy (ME) of the graph G as the sum of the absolute values of the zeros of the matching polynomial of G, and determine its basic properties. It is pointed out that the chemical applications of ME go back to the 1970s.

1. INTRODUCTION

In this paper we are concerned with undirected simple graphs, without multiple edges or self-loops. Let G be such a graph, and let n and m be the number of its vertices and edges, respectively.

By $m(G,k)$ we denote the number of k-matchings (= number of selections of k independent edges = number of k-element independent edge sets) of the graph G. Specifically, $m(G,1) = m$ and $m(G,k) = 0$ for $k > n/2$. It is both consistent and convenient to define $m(G,0) = 1$.

The matching polynomial of the graph G is defined as

$$\alpha(G) = \alpha(G,\lambda) = \sum_{k\geq 0} (-1)^k\, m(G,k)\, \lambda^{n-2k} \tag{1}$$

and its theory is well elaborated [5, 8, 11, 14]. For any graph G, all the zeros of $\alpha(G)$ are real–valued [5, 10, 11, 27].

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of a graph G, i. e., the eigenvalues of its $(0,1)$-adjacency matrix [6]. The energy of the graph G is then defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{2}$$

The theory of graph energy is nowadays well developed; its details can be found in the book [34] and reviews [17, 19]. An important result of this theory is the Coulson–type integral formula [13]

$$E(T) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{x^2} \ln \left[\sum_{k\geq 0} m(T,k)\, x^{2k} \right] dx \tag{3}$$

valid for any tree T (or, more generally, for any forest).

Formula (3) implies that the energy of a tree is a monotonically increasing function of any $m(T,k)$. In particular, if T' and T'' are two trees for which $m(T',k) \geq m(T'',k)$ holds for all $k \geq 1$, then $E(T') \geq E(T'')$. If, in addition, $m(T',k) > m(T'',k)$ for at least one k, then $E(T') > E(T'')$. Numerous results on the energy of trees were obtained using formula (3) and its consequences, see for instance the recent works [2, 28, 32, 33, 37].

2. A mathematical route to matching energy

The right hand side of Eq. (3) is well defined for any graph. Therefore, and bearing in mind the usefulness of formula (3) for the study of the energy of trees, we may consider it also for cycle–containing graphs. For such graphs, the right hand side of Eq. (3) is not the graph energy, but a quantity which we will call "*matching energy*".

Definition 1. Let G be a simple graph, and let $m(G,k)$ be the number of its k-matchings, $k = 0, 1, 2, \dots$. The matching energy of G is

$$\mathrm{ME} = \mathrm{ME}(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[\sum_{k \geq 0} m(G,k)\, x^{2k} \right] dx. \tag{4}$$

Knowing how formula (3) was obtained [4, 13, 20], and recalling the definition of graph energy, Eq. (2), we straightforwardly arrive at:

Theorem 1. *Let G be a simple graph, and let $\mu_1, \mu_2, \dots, \mu_n$ be the zeros of its matching polynomial. Then,*

$$\mathrm{ME}(G) = \sum_{i=1}^{n} |\mu_i|. \tag{5}$$

Eq. (5) could be considered as the definition of matching energy, in which case Eq. (4) would become a theorem.

3. A chemical route to matching energy

In the case of graphs representing conjugated molecules, the graph energy (E) is closely related to their total π-electron energy (E_π), as calculated within the Hückel molecular orbital approximation. In most cases, $E_\pi \equiv E$; for details see [12, 23].

In fact, if the eigenvalues of a (molecular) graph are ordered in a non-increasing manner, then [12, 23]

$$E_\pi = \begin{cases} 2 \sum\limits_{i=1}^{n/2} \lambda_i & \text{if } n \text{ is even,} \\ 2 \sum\limits_{i=1}^{(n-1)/2} \lambda_i + \lambda_{(n+1)/2} & \text{if } n \text{ is odd.} \end{cases} \tag{6}$$

The so defined E_π differs from the graph energy E only in the case of some non-bipartite graphs, and for chemically relevant graphs this difference is insignificant [23]. On the other hand, the definition (2) has many mathematical advantages over (6). For instance, for E, the Coulson–type integral formulas are applicable for all graphs, whereas for E_π it only applies to bipartite graphs. Whereas scores of mathematical results have been and are being obtained for E (see [34]), only a limited number of general mathematical results could be deduced for E_π (see [9]).

In theoretical chemistry, it has been established that a significant part of E_π comes from the presence of cycles in the carbon–atom skeleton of the underlying conjugated molecule. These cyclic effects are responsible for the stability or lack of stability of these molecules; for details see [7]. In order to "extract" the energy–effect of cycles, an acyclic reference needs be constructed. The difference between E_π and the energy of this reference is referred to as the "*resonance energy*" or "*delocalization energy*". Several resonance energies have been considered in the literature [23]. Of these, the so-called "*topological resonance energy*" (TRE) seems to have the best mathematical foundation. It was put forward in the 1970s, independently by two research groups [1, 21, 22]. Since then, scores of papers dealing with applications of TRE have appeared in the chemical literature.

The reference energy in the TRE approach is computed by neglecting the contributions of all cycles in the characteristic polynomial of the (molecular) graph G. By this, the characteristic polynomial reduces to the matching polynomial $\alpha(G)$, and the reference energy to the double sum of the positive zeros of $\alpha(G)$. The sum of all zeros of $\alpha(G)$ is zero. Therefore, the reference energy of the TRE method is equal to the sum of absolute values of all zeros of the matching polynomial, which is just the expression given by Eq. (5). Thus, we arrive at the simple relation

$$\mathrm{TRE}(G) = \mathrm{E}(G) - \mathrm{ME}(G). \tag{7}$$

This equation shows that the matching energy is a quantity of relevance for chemical applications. In view of this, and the fact that in the recent years a vast variety of energy–like graph invariants has been studied in the mathematical literature, it is somewhat surprising that until now no mathematical investigation of the matching energy has been undertaken. The present paper is aimed at contributing towards filling this gap.

4. Basic properties of the matching energy

From Definition 1 and Eq. (3) it immediately follows:

Theorem 2. *If the graph G is a forest, then its matching energy coincides with its energy.*

The integral on the right–hand side of Eq. (4) is increasing in all the coefficients $m(G, k)$. From this fact, one can readily deduce the extremal graphs for the matching energy. Since

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1) \tag{8}$$

holds for any edge e of the graph G, connecting the vertices u and v [8, 11, 14], we see that $m(G, k)$ can only increase when edges are added to a graph (and at least for $m(G, 1)$, the number increases strictly when this is done). From this observation we obtain the following theorem:

Theorem 3. *Let G be a graph and e one of its edges. Let $G - e$ be the subgraph obtained by deleting from G the edge e, but keeping all the vertices of G. Then*

$$\mathrm{ME}(G - e) < \mathrm{ME}(G).$$

Corollary 4. *Among all graphs on n vertices, the empty graph E_n without edges and the complete graph K_n have, respectively, minimum and maximum matching energy.*

Corollary 5. *The connected graph on n vertices having minimum matching energy is the star S_n.*

Proof. In view of Theorem 3, the connected graph with minimal ME must be a tree. By Theorem 2, trees have equal E– and ME-values. The fact that, among n-vertex trees, the star has minimal energy was established long time ago [13]. □

The matching energy of the empty graph is clearly 0, and the matching energy of the star, which equals its classical energy, is easily computed to be $\mathrm{ME}(S_n) = 2\sqrt{n-1}$. There does not seem to be a similarly simple expression for the maximum matching energy $\mathrm{ME}(K_n)$. The matching polynomial of the complete graph K_n is known to be a Hermite polynomial [5, 11], and the zeros of the Hermite polynomials are quite complicated. But of course it is desirable to know at least the order of magnitude of the maximum matching energy, which will be determined in the following section. Before that, however, let us continue our general considerations.

The quasi–order $\succ$, defined by

$$G \succ H \quad \Longleftrightarrow \quad m(G,k) \geq m(H,k) \text{ for all } k$$

has proved fundamental in the study of the graph energy, but it is also interesting in its own right. From the definition of the matching energy, it is clear that $G \succ H$ implies $\mathrm{ME}(G) \geq \mathrm{ME}(H)$. Hence a number of important techniques that are used to determine extremal graphs with respect to the graph energy and the Hosoya index (which is the sum of all the $m(G,k)$'s) can be applied to the matching energy as well. In particular, we have the following simple result.

Denote by $\mathcal{U}_n$ the set of all connected unicyclic graphs on n vertices. Let C_n be the n-vertex cycle, and let S_n^+ be the graph obtained by adding a new edge to the star S_n. Of course, $C_n\,,\ S_n^+ \in \mathcal{U}_n$.

Theorem 6. *If $G \in \mathcal{U}_n$, then*

$$\mathrm{ME}(S_n^+) \leq \mathrm{ME}(G) \leq \mathrm{ME}(C_n)$$

with equality if and only if $G \cong S_n^+$ and $G \cong C_n$, respectively.

Proof. In the following considerations we shall need the relation

$$m(G,2) = \binom{m}{2} - \sum_{i=1}^{n} \binom{d_i}{2}, \tag{9}$$

where d_i is the degree of the i-th vertex.

We start with the first inequality stated in Theorem 6. The graph S_n^+ has no three independent edges, and therefore $m(S_n^+,k) = 0$ for all $k \geq 3$. If $G \ncong S_n^+$, then by using Eq. (9) we can easily verify that $m(S_n^+,2) < m(G,2)$. For all graphs $G \in \mathcal{U}_n$, $m(G,1) = n$. This implies $\mathrm{ME}(S_n^+) < \mathrm{ME}(G)$ provided $G \in \mathcal{U}_n \setminus \{S_n^+\}$.

Let e be an edge of the graph G, belonging to its cycle and connecting the vertices u and v. Then $G-e$ is an n-vertex tree, and $G-u-v$ is an $(n-2)$-vertex forest. If $G \cong C_n$, then $G - e \cong P_n$ and $G-u-v \cong P_{n-2}$, where P_ℓ stands for the ℓ-vertex path.

It is known [13] that for any ℓ-vertex forest F_ℓ and for any value of k, $m(F_\ell,k) \leq m(P_\ell,k)$. Therefore,

$$m(G-e,k) \leq m(P_n,k) \quad \text{ and } \quad m(G-u-v,k-1) \leq m(P_{n-2},k-1).$$

Bearing in mind relation (8), we get

$$m(G,k) \leq m(P_n,k) + m(P_{n-2},k-1) = m(C_n,k),$$

i. e., $C_n \succ G$ and therefore $\mathrm{ME}(C_n) \geq \mathrm{ME}(G)$. If $G \ncong C_n$, then by using Eq. (9) it is easy to check that $m(C_n,2) > m(G,2)$. Consequently, $\mathrm{ME}(C_n) > \mathrm{ME}(G)$ provided $G \in \mathcal{U}_n \setminus \{C_n\}$. $\square$

Remark 1. The matching polynomial of the graph S_n^+ is $x^n - nx^{n-2} + (n-3)x^{n-4}$, hence we have

$$\begin{aligned}\mathrm{ME}(S_n^+) &= \sqrt{2n + 2\sqrt{n^2-4n+12}} + \sqrt{2n - 2\sqrt{n^2-4n+12}}\\ &= 2(\sqrt{n}+1) + O(n^{-1/2}).\end{aligned}$$

It is also not hard to prove that the zeros of the matching polynomial of C_n are $2\cos((2j-1)\pi/(2n))$, $j = 1, \ldots, n$, from which one derives

$$\mathrm{ME}(C_n) = \begin{cases} 2\csc\frac{\pi}{2n} & n \text{ even},\\ 2\cot\frac{\pi}{2n} & n \text{ odd},\end{cases}$$

and thus $\mathrm{ME}(C_n) = 4n/\pi + O(1/n)$. A similar formula holds for the path (which maximizes the matching energy among trees, since ME coincides with the "ordinary" energy in the case of trees):

$$\mathrm{ME}(P_n) = E(P_n) = \begin{cases} 2\csc\frac{\pi}{2n+2} - 2 & n \text{ even},\\ 2\cot\frac{\pi}{2n+2} - 2 & n \text{ odd}.\end{cases}$$

By Corollary 5 we know which connected bipartite graph has minimal matching energy. From Theorem 3 it is evident that the bipartite graph with maximal ME must be one of the complete bipartite graphs $K_{a,b}$.

Theorem 7. *The bipartite graph on n vertices having maximum matching energy is $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$.*

Proof. Let $K_{a,b}$ be the complete bipartite graph with $a+b$ vertices, and let $a < b$. In order to prove Theorem 7 it is sufficient to demonstrate that $K_{a+1,b-1} \succ K_{a,b}$. For this, we use the identity [5, 14]

$$m(G,k) = m(G-v,k) + \sum_u m(G-u-v,k-1)$$

where the summation goes over all vertices u adjacent to the vertex v. Special cases of the above relation are:

$$\begin{aligned} m(K_{a,b},k) &= m(K_{a,b-1},k) + a\,m(K_{a-1,b-1},k-1),\\ m(K_{a+1,b-1},k) &= m(K_{a,b-1},k) + (b-1)\,m(K_{a,b-2},k-1).\end{aligned}$$

If $k > a+1$, then both are zero. Otherwise, we get

$$\begin{aligned} m(K_{a+1,b-1},k) - m(K_{a,b},k) &= (b-1)\,m(K_{a,b-2},k-1) - a\,m(K_{a-1,b-1},k-1)\\ &\geq a\left[m(K_{a,b-2},k-1) - m(K_{a-1,b-1},k-1)\right]\\ &\geq a(a-1)\left[m(K_{a-1,b-3},k-2) - m(K_{a-2,b-2},k-2)\right]\\ &\cdots\\ &\geq a(a-1)\cdots(a-k+2)\left[m(K_{a+2-k,b-k},1) - m(K_{a+1-k,b+1-k},1)\right]\\ &= a(a-1)\cdots(a-k+2)(b-a-1) \geq 0.\end{aligned}$$

This implies that $m(K_{\lfloor n/2\rfloor,\lceil n/2\rceil},k) \geq m(K_{a,b},k)$ for all k and all $a+b=n$. Since $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ has greatest number of edges among the n-vertex complete bipartite graphs, $m(K_{\lfloor n/2\rfloor,\lceil n/2\rceil},1) > m(K_{a,b},1)$ for all $(a,b) \neq (\lfloor n/2\rfloor, \lceil n/2\rceil)$ and we are done. □

In the 1980s one of the present authors established a number of relations of the type $G \succ H$ [15, 16, 18, 24, 25, 38]. Each such result could now be re-interpreted as a statement on matching energy. Two characteristic results of this kind are the following two lemmas:

Lemma 8 ("Sliding"). *Let G be a connected graph with at least two vertices, and let u be one of its vertices. Denote by $P(n, k, G, u)$ the graph obtained by identifying u with the vertex v_k of a simple path $v_1, v_2, \ldots, v_n$. Write $n = 4p + i$, $i \in \{1, 2, 3, 4\}$, and $\ell = \lfloor (i-1)/2 \rfloor$. Then the inequalities*

$$\begin{aligned}\mathrm{ME}(P(n,2,G,u)) < \mathrm{ME}(P(n,4,G,u)) < \cdots < \mathrm{ME}(P(n,2p+2\ell,G,u)) \\ < \mathrm{ME}(P(n,2p+1,G,u)) < \cdots < \mathrm{ME}(P(n,3,G,u)) < \mathrm{ME}(P(n,1,G,u))\end{aligned}$$

hold.

Lemma 9 ("Ironing"). *Suppose that G is a connected graph and T an induced subgraph of G such that T is a tree and T is connected to the rest of G only by a cut vertex v. If T is replaced by a star of the same order, centered at v, then the matching energy decreases (unless T is already such a star). If T is replaced by a path, with one end at v, then the matching energy increases (unless T is already such a path).*

To conclude this section, let us note that the matching energy has the (desirable) property that

$$\mathrm{ME}(G_1 \cup G_2) = \mathrm{ME}(G_1) + \mathrm{ME}(G_2)$$

if G_1 and G_2 are disjoint. The following simple result slightly strengthens this property by showing that an inequality holds in general:

Proposition 10. *Suppose that G_1 and G_2 are graphs on the same set of vertices, but with disjoint edge sets. Then the union of G_1 and G_2 satisfies*

$$\max(\mathrm{ME}(G_1), \mathrm{ME}(G_2)) \leq \mathrm{ME}(G_1 \cup G_2) \leq \mathrm{ME}(G_1) + \mathrm{ME}(G_2).$$

Equality in the first inequality holds if and only if at least one of the two graphs is empty. Equality in the second inequality holds if and only if no edge of G_1 is adjacent to an edge in G_2.

Proof. The first inequality is trivial since G_1 and G_2 are subgraphs of $G_1 \cup G_2$. For the second part, note that every matching of $G_1 \cup G_2$ can be decomposed in a unique way into a matching of G_1 and a matching of G_2, but the union of a matching in G_1 and a matching in G_2 is not necessarily again a matching. Hence we have

$$m(G_1 \cup G_2, k) \leq \sum_{j=0}^{k} m(G_1, j) m(G_2, k-j),$$

and we deduce

$$\sum_{k \geq 0} m(G_1 \cup G_2, k) x^k \leq \left(\sum_{k \geq 0} m(G_1, k) x^k \right) \left(\sum_{k \geq 0} m(G_2, k) x^k \right)$$

for any nonnegative x. The inequality now follows directly from the definition of the matching energy. At least one of the inequalities is strict, unless none of the edges of G_1 is adjacent to an edge of G_2. □

In particular, we have the following immediate consequence:

Corollary 11. *For any graph G and any edge e of G,*

$$\mathrm{ME}(G-e) \leq \mathrm{ME}(G) \leq \mathrm{ME}(G-e)+2.$$

Combining this with Theorem 6 and the remark thereafter, we easily obtain the following:

Corollary 12. *The minimum and maximum of the matching energy for graphs of order n with fixed cyclomatic number k are $2\sqrt{n}+O(1)$ and $4n/\pi+O(1)$ respectively, where the implied constants only depend on k.*

5. Asymptotic results

As mentioned earlier, there does not seem to be a simple formula for the matching energy of a complete graph, which is the maximum matching energy of any graph of given order. However, we can provide a fairly precise asymptotic formula for $\mathrm{ME}(K_n)$:

Theorem 13. *The matching energy of the complete graph K_n is asymptotically equal to $8/(3\pi)\cdot n^{3/2}$. More precisely,*

$$\mathrm{ME}(K_n) = \frac{8\,n^{3/2}}{3\pi} + O(n). \tag{10}$$

Proof. We use the exponential generating function of the auxiliary polynomial

$$M_n(x) = \sum_{k\geq 0} m(K_n,k)\,x^{2k}.$$

Since

$$m(K_n,k) = m(K_{n-1},k) + (n-1)\,m(K_{n-2},k-1),$$

we have

$$M_n(x) = M_{n-1}(x) + (n-1)\,x^2\,M_{n-2}(x).$$

This translates to a differential equation for the exponential generating function $A(x,z) = \sum_{n\geq 0} M_n(x) z^n/n!$:

$$\frac{\partial A(x,z)}{\partial z} = (1+x^2 z)\,A(x,z)$$

and thus $A(x,z) = \exp\left(z + \frac{x^2 z^2}{2}\right)$, which means that

$$M_n(x) = n!\,[z^n]\exp\left(z + \frac{x^2\,z^2}{2}\right) = \sum_{k=0}^{\lfloor n/2\rfloor} \frac{n!\,x^{2k}}{k!\,(n-2k)!\,2^k},$$

an identity that can also be derived easily by a direct counting argument. This allows us to use the saddle point method to determine the asymptotic behavior of $M_n(x)$ as $n\to\infty$. Before that, we apply a change of variables to the integral representation

$$\mathrm{ME}(K_n) = \frac{2}{\pi}\int_0^\infty x^{-2}\ln M_n(x)\,dx.$$

The substitution $x = \sqrt{(1-y)/(y^2 n)}$ might seem contrived, but it simplifies the following calculation. We obtain

$$\mathrm{ME}(K_n) = \frac{\sqrt{n}}{\pi} \int_0^1 \frac{2-y}{(1-y)^{3/2}} \ln M_n\left(\sqrt{\frac{1-y}{y^2\, n}}\right) dy.$$

Now we estimate the integrand, which is done by distinguishing three cases depending on the value of y.

Case 1: $y \le n^{-3/4}$. Then the trivial bound $[z^n]F(z) \le r^{-n}F(r)$, which holds for any power series $F(z)$ with nonnegative coefficients and any $r > 0$, yields

$$\begin{aligned} 1 \le M_n\left(\sqrt{\frac{1-y}{y^2\, n}}\right) &= n!\,[z^n] \exp\left(z + \frac{(1-y)z^2}{2n\, y^2}\right) \\ &\le n!\,(ny)^{-n} \exp\left(ny + \frac{(1-y)n^2\, y^2}{2n\, y^2}\right) \\ &= n!\,(ny)^{-n} \exp\left(\frac{(1+y)n}{2}\right). \end{aligned}$$

Together with Stirling's formula, this implies $0 \le \ln M_n \le n(-\ln y + O(1))$. Hence the contribution of this case to the integral is at most

$$\frac{n^{3/2}}{\pi} \int_0^{n^{-3/4}} \frac{2-y}{(1-y)^{3/2}} (-\ln y + O(1))\, dy = O\left(n^{3/2} \cdot n^{-3/4} \ln n\right) = O\left(n^{3/4} \ln n\right).$$

Case 2: $y \ge 1 - 1/n$. Then

$$x = \sqrt{\frac{1-y}{y^2\, n}} \le \frac{1}{yn} \le \frac{1}{n-1} \le \frac{2}{n}$$

for $n \ge 2$. Now we use the explicit representation of $M_n(x)$:

$$1 \le M_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n!\, x^{2k}}{k!(n-2k)!\, 2^k} \le \sum_{k=0}^{\infty} \frac{n^{2k}\, x^{2k}}{k!\, 2^k} = e^{n^2\, x^2/2}.$$

This implies $0 \le \ln M_n(x) \le n^2\, x^2/2$, and so the contribution to the integral is at most

$$\frac{\sqrt{n}}{\pi} \int_{1-1/n}^{1} \frac{2-y}{(1-y)^{3/2}} \cdot \frac{n^2\,(1-y)}{2y^2\, n}\, dy = \frac{n^{3/2}}{2\pi} \int_{1-1/n}^{1} \frac{2-y}{y^2\sqrt{1-y}}\, dy = \frac{n^2}{\pi(n-1)} = O(n).$$

Case 3: $n^{-3/4} \le y \le 1 - 1/n$. Then the residue theorem yields

$$\begin{aligned} A_n(y) = M_n\left(\sqrt{\frac{1-y}{y^2\, n}}\right) &= n!\,[z^n] \exp\left(z + \frac{(1-y)z^2}{2n\, y^2}\right) \\ &= \frac{n!}{2\pi i} \oint_{\mathcal{C}} z^{-n-1} \exp\left(z + \frac{(1-y)z^2}{2n\, y^2}\right) dz \end{aligned}$$

for any closed contour $\mathcal{C}$ around 0. We choose $\mathcal{C}$ to be the circle of radius ny around 0, the point being that it passes through the saddle point. The change of variables $z = ny\, e^{it}$ yields

$$A_n(y) = \frac{n!\,(ny)^{-n}}{2\pi} \int_{-\pi}^{\pi} \exp\left(nye^{it} + \frac{n(1-y)e^{2it}}{2} - int\right) dt.$$

Now we split this integral into a central part ($|t| \leq n^{-2/5}$) and the rest. Let us first focus on the central part. Taylor expansion yields

$$\begin{aligned} nye^{it} + \frac{n(1-y)e^{2it}}{2} - int &= n\left(\frac{1+y}{2} - \frac{2-y}{2}\,t^2 + O(|t|^3)\right) \\ &= \frac{(1+y)n}{2} - \frac{(2-y)n\,t^2}{2} + O(n^{-1/5}). \end{aligned}$$

Note that the linear term vanishes as a result of our choice of $\mathcal{C}$. This gives us

$$\int_{-n^{-2/5}}^{n^{-2/5}} \exp\left(nye^{it} + \frac{n(1-y)e^{2it}}{2} - int\right) dt$$

$$= \exp\left(\frac{(1+y)n}{2}\right)\left(\int_{-n^{-2/5}}^{n^{-2/5}} \exp\left(-\frac{(2-y)n\,t^2}{2}\right) dt\right)\left(1 + O(n^{-1/5})\right).$$

The remaining integral is easy to estimate:

$$\begin{aligned} \int_{-n^{-2/5}}^{n^{-2/5}} \exp\left(-\frac{(2-y)n\,t^2}{2}\right) dt &= \sqrt{\frac{2\pi}{(2-y)n}} - 2\int_{n^{-2/5}}^{\infty} \exp\left(-\frac{(2-y)n\,t^2}{2}\right) dt \\ &= \sqrt{\frac{2\pi}{(2-y)n}} + O\left(\int_{n^{-2/5}}^{\infty} \exp\left(-\frac{n^{3/5}\,t}{2}\right) dt\right) \\ &= \sqrt{\frac{2\pi}{(2-y)n}} + O\left(\exp\left(-\frac{n^{1/5}}{2}\right)\right). \end{aligned}$$

Hence the contribution of the central part is

$$\sqrt{\frac{2\pi}{(2-y)n}}\exp\left(\frac{(1+y)n}{2}\right)\left(1 + O(n^{-1/5})\right)$$

and we are left with the tails, i. e., $|t| \geq n^{-2/5}$. Note that

$$\left|\exp\left(ny\,e^{it} + \frac{n(1-y)}{2}\cdot e^{2it} - int\right)\right| = \exp\left(ny\cos t + \frac{n(1-y)}{2}\cos 2t\right).$$

If now $|t| \geq \pi/2$, then $\cos t \leq 0$, and thus

$$\left|\exp\left(ny\,e^{it} + \frac{n(1-y)}{2}\cdot e^{2it} - int\right)\right| \leq \exp\left(\frac{(1-y)n}{2}\right) \leq \exp\left(\frac{(1+y)n}{2} - n^{1/4}\right)$$

since $y \geq n^{-3/4}$. If, on the other hand, $|t| \leq \pi/2$, then we can use the inequalities $\cos 2t \leq 1 - 8t^2/\pi^2$ and $\cos t \leq 1 - 4t^2/\pi^2$ to obtain

$$\left|\exp\left(ny\,e^{it} + \frac{n(1-y)}{2} \cdot e^{2it} - int\right)\right| \leq \exp\left(\frac{(1+y)n}{2} - \frac{4n\,t^2}{\pi^2}\right) \leq \exp\left(\frac{(1+y)n}{2} - \frac{4\,n^{1/5}}{\pi^2}\right).$$

Hence the tails only contribute

$$O\left(\exp\left(\frac{(1+y)n}{2} - \frac{4\,n^{1/5}}{\pi^2}\right)\right)$$

so that

$$A_n(y) = \frac{n!\,(ny)^{-n}}{2\pi} \cdot \sqrt{\frac{2\pi}{(2-y)n}}\,\exp\left(\frac{(1+y)n}{2}\right)\left(1 + O(n^{-1/5})\right),$$

and this asymptotic formula holds uniformly in y. Applying the Stirling formula, we find

$$A_n(y) = \frac{1}{\sqrt{2-y}}\,\exp\left(\left(\frac{y-1}{2} - \ln y\right)n\right)\left(1 + O(n^{-1/5})\right)$$

uniformly in y. Thus

$$\ln A_n(y) = \left(\frac{y-1}{2} - \ln y\right)n + O(1)$$

and we can finally evaluate the third part of our main integral:

$$\begin{aligned}
&\frac{\sqrt{n}}{\pi}\int_{n^{-3/4}}^{1-1/n} \frac{2-y}{(1-y)^{3/2}} \ln M_n\left(\sqrt{\frac{1-y}{y^2\,n}}\right) dy \\
&= -\frac{n^{3/2}}{\pi}\int_{n^{-3/4}}^{1-1/n} \left(\frac{2-y}{2\sqrt{1-y}} + \frac{(2-y)\ln y}{(1-y)^{3/2}}\right) dy + O\left(\sqrt{n}\int_{n^{-3/4}}^{1-1/n} \frac{2-y}{(1-y)^{3/2}}\,dy\right) \\
&= -\frac{n^{3/2}}{\pi}\int_0^1 \left(\frac{2-y}{2\sqrt{1-y}} + \frac{(2-y)\ln y}{(1-y)^{3/2}}\right) dy + O\left(n^{3/2}\int_0^{n^{-3/4}} |\ln y|\,dy\right) \\
&\quad + O\left(n^{3/2}\int_{1-1/n}^{1} (1-y)^{-1/2}\,dy\right) + O\left(\sqrt{n}\int_0^{1-1/n} (1-y)^{-3/2}\,dy\right) \\
&= \frac{8\,n^{3/2}}{3\pi} + O(n).
\end{aligned}$$

Putting the three parts together, we finally arrive at the asymptotic formula (10). □

It was shown in [36] that almost all graphs have an energy of order $\Theta(n^{3/2})$. This is also true for the matching energy. In view of the upper bound we just determined, it is sufficient to prove a lower bound of order $n^{3/2}$:

Theorem 14. *Consider random graphs $G_{n,p}$ of order n with fixed probability $p \in (0,1)$. Then*

$$\mathrm{ME}(G_{n,p}) \geq \frac{\sqrt{p}}{\pi} n^{3/2} + O(\sqrt{n} \ln n)$$

holds asymptotically almost surely.

Proof. We make use of a result of Janson [29] stating that the number of perfect matchings of a random graph $G_{n,p}$ asymptotically follows a log-normal distribution (if n is even). For our purposes, it is sufficient to know that

$$\ln m(G_{n,p}, n/2) - \ln \mathbb{E}(m(G_{n,p}, n/2)) = O(\omega(n))$$

with probability tending to 1 for any function ω such that $\lim_{n\to\infty} \omega(n) = \infty$. Since

$$\ln \mathbb{E}(m(G_{n,p}, n/2)) = \ln\left((n-1)!!p^{n/2}\right) = \frac{n}{2}(\ln n - 1 + \ln p) + O(\ln n),$$

we obtain

$$\begin{aligned}
\mathrm{ME}(G_{n,p}) &\geq \frac{2}{\pi}\int_{(pn)^{-1/2}}^{\infty} \frac{dx}{x^2} \ln\left(m(G_{n,p}, n/2)x^n\right) \\
&= \frac{n}{\pi}\int_{(pn)^{-1/2}}^{\infty} \frac{dx}{x^2}(\ln n - 1 + \ln p + 2\ln x) + O\left(\ln n \int_{(pn)^{-1/2}}^{\infty} \frac{dx}{x^2}\right) \\
&= \frac{\sqrt{p}}{\pi} n^{3/2} + O(\sqrt{n}\ln n)
\end{aligned}$$

with probability tending to 1. If n is odd, we get the same lower bound by simply removing one of the vertices. ☐

Remark 2. Note that the expectation of $m(G_{n,p}, k)$ is

$$\mathbb{E}(m(G_{n,p}, k)) = \frac{n!p^k}{2^k k!(n-2k)!},$$

hence it is tempting to conjecture that

$$\begin{aligned}
\mathbb{E}(\mathrm{ME}(G_{n,p})) &\sim \frac{2}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln \sum_{k\geq 0} \frac{n!p^k x^{2k}}{2^k k!(n-2k)!}\, dx \\
&= \frac{2\sqrt{p}}{\pi}\int_0^{\infty} \frac{1}{y^2} \ln \sum_{k\geq 0} \frac{n! y^{2k}}{2^k k!(n-2k)!}\, dy = \sqrt{p}\,\mathrm{ME}(K_n) \sim \frac{8\sqrt{p}}{3\pi} \cdot n^{3/2},
\end{aligned}$$

perhaps even that $n^{-3/2}\mathbb{E}(\mathrm{ME}(G_{n,p})) \to 8\sqrt{p}/(3\pi)$ asymptotically almost surely, but of course it is not at all clear whether expectation, limit, logarithm and integral can really be interchanged in this way.

6. Bounds for the matching energy

The zeros of the matching polynomial satisfy the relations

$$\sum_{i=1}^{n} \mu_i^2 = 2m \qquad \text{and} \qquad \sum_{i<j} \mu_i\, \mu_j = -m$$

which are fully analogous to the relations obeyed by the graph eigenvalues, namely

$$\sum_{i=1}^{n} \lambda_i^2 = 2m \qquad \text{and} \qquad \sum_{i<j} \lambda_i \, \lambda_j = -m. \tag{11}$$

By means of Eqs. (11) certain simple bounds for the graph energy have been deduced [3,35]. In a fully analogous manner we can prove the following bounds for the matching energy:

Theorem 15. (a) *Let G be a graph with n vertices and m edges. Then $\mathrm{ME}(G) \le \sqrt{2mn}$. Equality holds if and only if either $m = 0$ or G is regular of degree 1 (i. e., G consists of m copies of K_2).*
(b) *Let G be a graph with m edges. Then $2\sqrt{m} \le \mathrm{ME}(G) \le 2m$. Equality $\mathrm{ME}(G) = 2\sqrt{m}$ holds if and only if G consists of a star on $m+1$ vertices or a single K_3 (if $m = 3$) and an arbitrary number of isolated vertices. Equality $\mathrm{ME}(G) = 2m$ holds if and only G consists of m copies of K_2 and an arbitrary number of isolated vertices.*
(c) *Let G be a graph with n vertices consisting of p components, none of which is an isolated vertex. Then $\mathrm{ME}(G) \ge 2\sqrt{n + p(p-2)}$. Equality holds if and only if G is regular of degree 1.*

Remark 3. The second part of (b) also follows directly from Proposition 10.

In what follows we offer a tighter estimate for ME. Let the zeros of the matching polynomial of the graph G be labelled so that

$$\mu_1 \ge \mu_2 \ge \cdots \ge \mu_L > 0 \ge \mu_{L+1} \ge \cdots \ge \mu_n \, .$$

Then, as well known [5,11,14], $\mu_{n-i+1} = -\mu_i$ for $i = 1, 2, \ldots, L$. In addition, if $2L < n$, then $\mu_i = 0$ for $L + 1 \le i \le n - L$.

From Eq. (1) we see that L is the size of the maximum matching(s) of G, which means that $m(G, L) > 0$ and $m(G, L + 1) = 0$. It now immediately follows that

$$\sum_{i=1}^{L} \mu_i = \frac{1}{2}\,\mathrm{ME}(G); \qquad \sum_{i=1}^{L} \mu_i^2 = m; \qquad \prod_{i=1}^{L} \mu_i = \sqrt{m(G,L)} \, . \tag{12}$$

Theorem 16. *The matching energy of a graph G with m edges and maximum matchings of size L is bounded as:*

$$2\sqrt{m + L(L-1)\, m(G,L)^{1/L}} \le \mathrm{ME}(G) \le 2\sqrt{(L-1)m + L\, m(G,L)^{1/L}} \, . \tag{13}$$

Proof. Let $x_1, x_2, \ldots, x_N$ be non-negative real numbers, and let

$$\mathcal{A} = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad \text{and} \qquad \mathcal{G} = \left(\prod_{i=1}^{N} x_i \right)^{1/N}$$

be, respectively, their arithmetic and geometric means. As well known, $\mathcal{A} \ge \mathcal{G}$. The difference of these two means is bounded as [30]:

$$\frac{1}{N(N-1)} \sum_{i<j} \left(\sqrt{x_i} - \sqrt{x_j} \right)^2 \le \mathcal{A} - \mathcal{G} \le \frac{1}{N} \sum_{i<j} \left(\sqrt{x_i} - \sqrt{x_j} \right)^2 . \tag{14}$$

Choosing $N = L$, setting $x_i = \mu_i^2,\ i = 1, 2, \dots, L$, and bearing in mind the relations (12), we obtain

$$\mathcal{A} = \frac{1}{L}\sum_{i=1}^{L}\mu_i^2 = \frac{m}{L}, \tag{15}$$

$$\mathcal{G} = \left(\prod_{i=1}^{L}\mu_i^2\right)^{1/L} = \left(\sqrt{m(G,L)}\right)^{2/L} = m(G,L)^{1/L}, \tag{16}$$

$$\sum_{i<j}\left(\sqrt{x_i} - \sqrt{x_j}\right)^2 = \frac{1}{2}\sum_{i=1}^{L}\sum_{j=1}^{L}\left(\mu_i^2 + \mu_j^2 - 2\,\mu_i\,\mu_j\right)$$

$$= L\sum_{i=1}^{L}\mu_i^2 - \left(\sum_{i=1}^{L}\mu_i\right)^2 = L\,m - \frac{\mathrm{ME}(G)^2}{4}. \tag{17}$$

Substituting (15)–(17) back into (14) we arrive at the estimates (13). □

Equality on both sides of (13) is attained if either $m = 0$ (in which case we have $L = 0$) or G consists of m copies of K_2 and an arbitrary number of isolated vertices (in which case $L = m$ and $m(G, L) = 1$).

For graphs with even number of vertices and $K = m(G, n/2)$ perfect matchings, by choosing $N = n/2$ and setting $x_i = \mu_i^2$, $i = 1, 2, \dots, n/2$, we get the following weaker variant of Theorem 16:

Theorem 17. *If the graph G has n vertices (n even), and $K \geq 0$ perfect matchings, then*

$$\sqrt{4m + n(n-2)\,K^{2/n}} \leq \mathrm{ME}(G) \leq \sqrt{2(n-2)m + 2n\,K^{2/n}}\ . \tag{18}$$

If $K > 0$, then equality on both sides of (18) holds if G is regular of degree 1.

If $K = 0$, then the inequalities (18) reduce to

$$2\sqrt{m} \leq \mathrm{ME}(G) \leq \sqrt{2(n-2)m}\ .$$

The equality $\mathrm{ME}(G) = 2\sqrt{m}$ has already been considered in Theorem 15. Equality $\mathrm{ME}(G) = \sqrt{2(n-2)m}$ is attained if and only if G consists of m copies of K_2 and two isolated vertices.

7. Conclusion

We have seen that many properties of the matching energy are analogous to those of the "ordinary" graph energy. However, there are some notable differences, such as the monotonicity property in Theorem 3, which trivially gave us the extremal graphs, while the structure of graphs maximizing the energy is much more complicated [26, 31].

Let us conclude this paper with a question:

Question. Is it true that the matching energy of a graph G coincides with its energy if and only if G is a forest?

It true, this statement would considerably strengthen Theorem 2.

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