MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 681-688

ISSN 0340 - 6253

On Almost–Equienergetic Graphs

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(Received March 17, 2013)

Abstract

Two graphs are said to be equienergetic if their energies are equal. In the paper *MATCH Commun. Math. Comput. Chem.* **61** (2009) 451–461 the concept of *almost-equienergetic* graphs was put forward, based on the observation that in some cases the (non-zero) difference between the energies of two graphs is very small. We now estimate the minimal value of this difference.

1 Introduction

Let G be a graph of order n and let its eigenvalues (i.e., the eigenvalues of the $(0,1)$-adjacency matrix of G) be $\lambda_1, \lambda_2, \ldots, \lambda_n$. The *energy* of G is defined as

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

For details on the theory of graph energy see the reviews [7, 8, 10], the book [17], and the references cited therein. Two graphs G_a and G_b are said to be *equienergetic* if the condition $E(G_a) - E(G_b) = 0$ is satisfied. This concept was introduced in 2004, independently by Balakrishnan [1] and Brankov et al. [2]. Since then, numerous pairs, triplets, and larger families of equienergetic graphs have been discovered and/or constructed [5,9,11–16,18–23].

Performing a computer–aided search for equienergetic trees [18], it was noticed that there exist pairs of trees for which the difference $E(G_a) - E(G_b)$ is remarkably small. A characteristic example of this kind is depicted in Fig. 1.

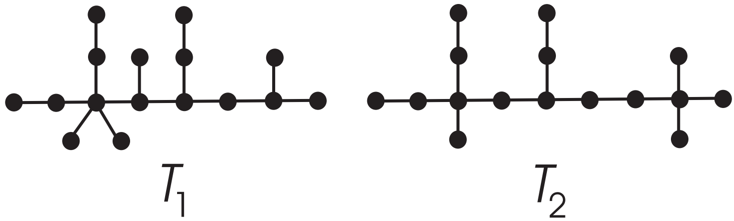

Fig. 1. Two trees whose energies differ only slightly: $E(T_1) = 18.090756640280765\ldots$, $E(T_2) = 18.090756641775140\ldots$.

Based on this observation, the concept of *almost–equienergetic* graphs was conceived [18]. However, a rigorous definition of almost–equienergeticity could not be given. In [18] we read:

... There also exist trees whose energies are different, but remarkably close. These we refer to as almost–equienergetic. ... What "remarkably close" means for the energy of two graphs is a theme for debate. ... We tentatively and to a great degree arbitrarily call two graphs G_a and G_b almost–equienergetic if $0 < |E(G_a) - E(G_b)| < 10^{-8}$.

In this note we show that the limit value 10^{-8} is indeed arbitrary and unjustified, and offer arguments in favor of the possibility that the difference $E(G_a) - E(G_b)$ can become much smaller.

2 Preparatory considerations

Throughout this paper we will consider bipartite graphs. The characteristic polynomial of a bipartite graph G of order n is of the form [3]

$$\phi(G,\lambda) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \, b(G,k) \, \lambda^{n-2k} \tag{1}$$

where $b(G,0) = 1$ and $b(G,k) \geq 0$ for all k , $1 \leq k \leq \lfloor n/2 \rfloor$.

Let thus G_a and G_b be two bipartite graphs of order n_a and n_b, respectively. According to a classical result by Coulson and Jacobs [4], if $n_a = n_b$, then

$$E(G_a) - E(G_b) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\phi(G_a\,,\, ix)}{\phi(G_b\,,\, ix)}\, dx$$

where $i = \sqrt{-1}$. If $n_a < n_b$, then a slightly modified form of the above integral expression applies:

$$E(G_a) - E(G_b) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{(i\,x)^{n_b - n_a}\, \phi(G_a\,,\, ix)}{\phi(G_b\,,\, ix)}\, dx\ .$$

In both cases, in view of Eq. (1),

$$E(G_a) - E(G_b) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\sum\limits_{k \geq 0} b(G_a, k)\, x^{2(m-k)}}{\sum\limits_{k \geq 0} b(G_b, k)\, x^{2(m-k)}}\, dx \tag{2}$$

where $m = \left\lfloor \frac{1}{2} \max\{n_a, n_b\} \right\rfloor$.

Bearing in mind Eq. (2), we see that without loss of generality it may be assumed that the graphs G_a and G_b have equal number n of vertices, and that $n = 2m$. If so, then replacing $b(G_a, k)$ by a_{2k} and $b(G_b, k)$ by b_{2k}, we get

$$E(G_a) - E(G_b) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{P(x)}{Q(x)}\, dx \tag{3}$$

with

$$\begin{aligned} P(x) &= x^n + a_2\, x^{n-2} + a_4\, x^{n-4} + \cdots + a_n = \sum_{k=0}^{m} a_{2k}\, x^{n-2k} \quad , \quad a_0 = 1 \\ Q(x) &= x^n + b_2\, x^{n-2} + b_4\, x^{n-4} + \cdots + b_n = \sum_{k=0}^{m} b_{2k}\, x^{n-2k} \quad , \quad b_0 = 1\ . \end{aligned}$$

In what follows, by investigating the integral

$$\mathcal{I} = \int_0^{+\infty} \ln \frac{P(x)}{Q(x)}\, dx \tag{4}$$

we establish some results relevant for the almost–equienergeticity concept.

3 Main result

Let $n = 2m\ ,\ m \in \mathbb{N}$, and

$$\begin{aligned} P(x) &= x^n + a_2\, x^{n-2} + a_4\, x^{n-4} + \cdots + a_n = \sum_{k=0}^{m} a_{2k}\, x^{n-2k} \quad , \quad a_0 = 1 \\ Q(x) &= x^n + b_2\, x^{n-2} + b_4\, x^{n-4} + \cdots + b_n = \sum_{k=0}^{m} b_{2k}\, x^{n-2k} \quad , \quad b_0 = 1 \end{aligned}$$

where $a_i, b_i \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$ and $b_i \leq a_i$. Let $\mathcal{I}$ be given by Eq. (4).

Since $\lim\limits_{n\to+\infty} \dfrac{P(x)}{Q(x)} = 1$ and $\ln x$ is a continuous function on $(0, +\infty)$, integration by parts yields

$$\begin{aligned} \mathcal{I} &= x \ln \frac{P(x)}{Q(x)}\Bigg|_0^{+\infty} - \int_0^{+\infty} \frac{P'(x)\,Q(x) - Q'(x)\,P(x)}{P(x)\,Q(x)}\, x\, dx \\ &= \int_0^{+\infty} \frac{P(x)\,Q'(x) - P'(x)\,Q(x)}{P(x)\,Q(x)}\, x\, dx\ . \end{aligned} \tag{5}$$

Choose now the polynomials P and Q so that $a_i = b_i$ for all $i \neq n - i_0$ and $a_{n-i_0} = b_{n-i_0} + \ell$, for some $\ell \in \mathbb{N}$. Then

$$P(x) = Q(x) + \ell\, x^{i_0} \qquad \text{and} \qquad P'(x) = Q'(x) + \ell\, i_0\, x^{i_0 - 1}$$

and therefore

$$P(x)\,Q'(x) - P'(x)\,Q(x) = \ell\, x^{i_0-1}\big(x\,Q'(x) - i_0\,Q(x)\big)\ .$$

Substituting this back into (5), we get

$$\mathcal{I}_1 = \ell \int_0^{+\infty} \frac{x^{i_0}\big(x\,Q'(x) - i_0\,Q(x)\big)}{Q(x)\big(Q(x) + \ell\, x^{i_0}\big)}\, dx\ .$$

Consider now the polynomials $\widetilde{P}(x)$ and $\widetilde{Q}(x)$, such that $\widetilde{P}(x) = P(x) + \ell\, x^{i_0}$ and $\widetilde{Q}(x) = Q(x) + \ell\, x^{i_0}$, i.e., $\widetilde{P}(x) = Q(x) + 2\ell\, x^{i_0}$ and $\widetilde{Q}(x) = Q(x) + \ell\, x^{i_0}$. Then the corresponding integral is

$$\mathcal{I}_2 = \ell \int_0^{+\infty} \frac{x^{i_0}\big(x\,Q'(x) - i_0\,Q(x)\big)}{\big(Q(x) + x^{i_0}\big)\big(Q(x) + 2\ell\, x^{i_0}\big)}\, dx\ .$$

Evidently, $\mathcal{I}_2 < \mathcal{I}_1$.

Continuing this procedure, namely by increasing the coefficients a_{i_0} and b_{i_0} each time by $\ell \geq 1$, we get a decreasing sequence of integrals:

$$\mathcal{I}_t = \ell \int_0^{+\infty} \frac{x^{i_0}\big(x\,Q'(x) - i_0\,Q(x)\big)}{\big(Q(x)+(t-1)\,x^{i_0}\big)\big(Q(x)+t\ell\,x^{i_0}\big)}\,dx \quad , \quad t = 1,2,3,\dots \ .$$

In what follows we demonstrate that $\mathcal{I}_t$ tends to zero as $t \to \infty$.

Let n, the degree of the polynomials be fixed, and let the coefficients at x^{i_0} differ by $\ell \in \mathbb{N}$, i.e., $b_{n-i_0} + \ell = a_{n-i_0}$. For the sake of simplicity, we denote $b_{n-i_0} = b$. We show that for any $\varepsilon > 0$, the coefficient b can be determined so that the value of the integral (4) be less than ε.

Lemma 1. *For $k \geq 2$,*

$$\int_0^{+\infty} \frac{dx}{b+x^k} = b^{1/k-1}\,\frac{\pi}{k}\,\csc\frac{\pi}{k}\ . \tag{6}$$

Proof. For $\Re\,\nu > \Re\,\mu > 0$ it is known [6, formula 3.241. 2,p. 319] that

$$\int_0^{+\infty} \frac{x^{\mu-1}\,dx}{1+x^\nu} = \frac{\pi}{\nu}\,\csc\frac{\mu\pi}{\nu}\ . \tag{7}$$

In our case, $k \geq 2 > \mu = 1 > 0$, and so the integral on the left–hand side of (6) is transformed as:

$$\int_0^{+\infty} \frac{dx}{b+x^k} = \frac{1}{b}\int_0^{\infty} \frac{dx}{1+\big(b^{-1/k}x\big)^k} = \frac{b^{1/k}}{b}\int_0^{\infty} \frac{dt}{1+t^k}\ .$$

The right–hand side of (6) follows now directly from (7). □

Recall that $\csc x = 1/\sin x$.

Theorem 1. *Let $\ell \in \mathbb{N}$, $P(x) = Q(x) + \ell\,x^{i_0}$, $Q(x) = x^n + \cdots + b\,x^{i_0} + \cdots + b_n$, and $k = n - i_0$. Then for an arbitrary $\varepsilon > 0$, for all*

$$b \geq \left(\frac{\ell\,\pi\,\csc(\pi/k)}{\varepsilon\,k}\right)^{k/(k-1)} \tag{8}$$

the condition $\mathcal{I} < \varepsilon$ holds for the integral (4).

Proof. According to the given conditions,

$$\ln\frac{P(x)}{Q(x)} = \ln\frac{Q(x)+\ell\,x^{i_0}}{Q(x)} = \ln\left(1+\frac{\ell\,x^{i_0}}{Q(x)}\right)$$
$$\leq \frac{\ell\,x^{i_0}}{Q(x)} \leq \frac{\ell\,x^{\ell\,i_0}}{x^n+b\,x^{i_0}} = \frac{\ell}{x^k+b}\ .$$

Note that the first inequality is a consequence of the inequality $\ln(1+x) \leq x$ for $x \geq 0$, whereas the second of that fact that the value of a fraction increases when the nominator is decreased. Therefore,

$$\int\limits_0^{+\infty} \ln\frac{P(x)}{Q(x)}\,dx \leq \ell \int\limits_0^{+\infty} \frac{dx}{x^k+b}$$

which combined with Lemma 1 implies

$$\int\limits_0^{+\infty} \ln\frac{P(x)}{Q(x)}\,dx \leq \frac{\ell}{b^{(k-1)/k}}\,\frac{\pi}{k}\csc\frac{\pi}{k} \leq \varepsilon$$

whenever the parameter b satisfies the condition (8). □

* * * * *

At this point it should be noted that in the above considerations we were not "hunting" for pairs of polynomials $P(x)$ and $Q(x)$ with integer coefficients, for which the value of the integral $\mathcal{I}$, Eq. (4), assumes the smallest non-zero value. Even smaller values must be encountered if some coefficients of $Q(x)$ are set smaller and some other greater than the respective coefficients of $P(x)$. Therefore, Theorem 1 may be understood as the analysis of the simplest case. Yet, its main implications are certainly valid also in the general case.

4 A discrete–mathematical caveat

At the first glance, from Eq. (3) and Theorem 1 it follows that there are pairs of non-equienergetic (finite) graphs whose energies differ arbitrarily little. However, Theorem 1 should be interpreted in a bit more cautious manner. In Theorem 1 it is required that the coefficient b be sufficiently large. On the other hand, in graphs with a fixed value n of vertices, the coefficients of the characteristic polynomial cannot assume arbitrarily large values. For instance, for a bipartite graph with $n = 2m$ vertices and maximal vertex degree Δ, the coefficient $b(G,k)$ in Eq. (1) is bounded by above as

$$b(G,k) \leq \Delta^{2k} \binom{m}{k}$$

with equality if and only if G consists of m isolated edges.

Anyway, because the number of graphs with a fixed value n of vertices is finite, there exists a smallest non-zero value that the energy difference does assume, say ε_n. In other words, there are no two non-equienergetic graphs of order n, such that their energies differ by less than ε_n. Consequently, for any finite n, the energy difference cannot become arbitrarily small.

Therefore, Theorem 1 should be interpreted as an indication that the energy difference may be much smaller than the earlier proposed limit 10^{-8}. Since the coefficients of the characteristic polynomial rapidly increase with n, Theorem 1 also implies that very small (non-zero) energy differences are expected to be encountered at graphs with large n-values.

Acknowledgement. The first author was supported in part by the Serbian Ministry of Education, Science and Technological Development (grant No. 174015).

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