On Almost–Equienergetic Graphs

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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-equieenergetic 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 λ1, λ2, ..., λn. 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 Ga and Gb 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: $E(T_1) = 18.090756640280765 \ldots$, $E(T_2) = 18.090756641775140 \ldots$.](image)

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]

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

(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:

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

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

\[
E(G_a) - E(G_b) = \frac{2}{\pi} \int_0^{+\infty} \ln \sum_{k \geq 0} b(G_a,k) x^{2(m-k)} \sum_{k \geq 0} b(G_b,k) x^{2(m-k)} \, dx
\]  \( (2) \)

where \( m = \lfloor \frac{1}{2} \max\{n_a, n_b\} \rfloor \).

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

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

with

\[
P(x) = x^n + a_2 x^{n-2} + a_4 x^{n-4} + \cdots + a_n = \sum_{k=0}^{m} a_{2k} x^{n-2k} \quad , \quad a_0 = 1
\]

\[
Q(x) = x^n + b_2 x^{n-2} + b_4 x^{n-4} + \cdots + b_n = \sum_{k=0}^{m} b_{2k} x^{n-2k} \quad , \quad b_0 = 1.
\]

In what follows, by investigating the integral

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

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

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

\[
P(x) = x^n + a_2 x^{n-2} + a_4 x^{n-4} + \cdots + a_n = \sum_{k=0}^{m} a_{2k} x^{n-2k}, \quad a_0 = 1
\]

\[
Q(x) = x^n + b_2 x^{n-2} + b_4 x^{n-4} + \cdots + b_n = \sum_{k=0}^{m} b_{2k} x^{n-2k}, \quad b_0 = 1
\]

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 \( \lim_{n \to +\infty} P(x)/Q(x) = 1 \) and \( \ln x \) is a continuous function on \((0, +\infty)\), integration by parts yields

\[
\mathcal{I} = \left. x \ln \frac{P(x)}{Q(x)} \right|_0^{+\infty} - \int_0^{+\infty} \frac{P'(x) Q(x) - Q'(x) P(x)}{P(x) Q(x)} x \, dx
\]

\[
= \int_0^{+\infty} \frac{P(x) Q'(x) - P'(x) Q(x)}{P(x) Q(x)} x \, dx . \tag{5}
\]

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

\[
P(x) = Q(x) + \ell x^{i_0} \quad \text{and} \quad P'(x) = Q'(x) + \ell i_0 x^{i_0-1}
\]

and therefore

\[
P(x) Q'(x) - P'(x) Q(x) = \ell x^{i_0-1} \left( x Q'(x) - i_0 Q(x) \right) .
\]

Substituting this back into (5), we get

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

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

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

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:

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

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 $\varepsilon$.

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

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

**Proof.** For $\Re \nu > \Re \mu > 0$ it is known [6, formula 3.241.2, p. 319] that

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

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

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

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

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

the condition $\mathcal{I} < \varepsilon$ holds for the integral (4).
Proof. According to the given conditions,

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

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,

\[
\int_0^{+\infty} \ln \frac{P(x)}{Q(x)} \, dx \leq \ell \int_0^{+\infty} \frac{dx}{x^k + b}
\]

which combined with Lemma 1 implies

\[
\int_0^{+\infty} \ln \frac{P(x)}{Q(x)} \, dx \leq \frac{\ell}{b^{(k-1)/k}} \frac{\pi}{k} \csc \frac{\pi}{k} \leq \varepsilon
\]

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

\[
\square
\]

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 \(I\), 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-equienegetic (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 $\Delta$, 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 $\varepsilon_n$. In other words, there are no two non-equienergetic graphs of order $n$, such that their energies differ by less than $\varepsilon_n$. 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.

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References


