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Note on Conjugated Unicyclic Graphs with Minimal Energy[1]

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Abstract

The energy of a graph G is defined as the sum of the absolute values of all the eigenvalues of the graph. Let $U(k)$ denote the set of all unicyclic graphs of order $2k$ which have a perfect matching. $S_3^1(k)$ denotes the unicyclic graph on $2k$ vertices obtained from a triangle C_3 by attaching one pendant edge and $k-2$ paths of length 2 together to one of the vertices of C_3, and $S_4^1(k)$ denotes the unicyclic graph on $2k$ vertices obtained from a cycle C_4 by attaching one path P of length 2 to one of the four vertices of C_4 and then attaching $k-3$ paths of length 2 to the middle vertex of the path P. In the paper "X. Li, J. Zhang and B. Zhou, On unicyclic conjugated molecules with minimal energies, J. Math. Chem. 42 (2007) 729-740", the authors proved that either $S_3^1(k)$ or $S_4^1(k)$ is the graph with the minimal energy in $U(k)$. They remarked that computation result shows that the energy of $S_3^1(k)$ is greater than that of $S_4^1(k)$ for larger k. However they could not find a proper way to prove this, and finally they conjectured that $S_4^1(k)$ is the unique graph with minimal energy in $U(k)$. This short note is to give a confirmative proof to the conjecture.

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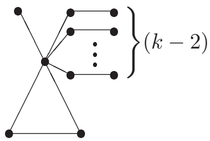
Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of a graph G of order n. The energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \ldots + |\lambda_n|$. A (molecular) graph is called *conjugated* if it has a perfect matching. Let $U(k)$ denote the set of all conjugated unicyclic graphs of order $2k$. $S_3^1(k)$ denotes the unicyclic graph on $2k$ vertices obtained from a triangle C_3 by attaching one pendant edge and $k-2$ paths of length 2 together to one of the vertices of C_3, and $S_4^1(k)$ denotes the unicyclic graph on $2k$ vertices obtained from a cycle C_4 by attaching one path P of length 2 to one of the four vertices of C_4 and then attaching $k-3$ paths of length 2 to the middle vertex of the path P. See Figure 1 for the graphs $S_3^1(k)$ and $S_4^1(k)$. For more information on graph energy we refer to [1], and for terminology and notations not defined here, we refer to [2] and the references therein.



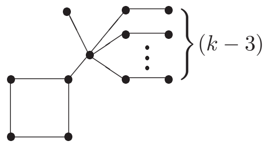


Figure 1. The graphs $S_3^1(k)$ and $S_4^1(k)$

In [2] the authors proved that either $S_3^1(k)$ or $S_4^1(k)$ is the graph with the minimal energy in $U(k)$. But, they could not determine which one of the two is smaller. They remarked that computation result shows that the energy of $S_3^1(k)$ is greater than that of $S_4^1(k)$ for $k \leq 100, 1000, 10000$. However, they could not find a proper way to prove this, and at the end of paper [2] they proposed a conjecture that $S_4^1(k)$ *is the unique graph with the minimal energy in* $U(k)$. In this short note we will give a confirmative proof to the conjecture.

By easy calculation or from Lemma 11 of [2], we have the following characteristic polynomials for $S_3^1(k)$ and $S_4^1(k)$:

$$\phi(S_3^1(k), \lambda) = (\lambda^2 - 1)^{k-2}(\lambda^4 - (k+4)\lambda^2 - 2\lambda + 1),$$
$$\phi(S_4^1(k), \lambda) = \lambda^2(\lambda^2 - 1)^{k-4}(\lambda^6 - (k+4)\lambda^4 + 4k\lambda^2 - 6).$$

Theorem 1. $S_4^1(k)$ *is the graph with minimal energy in* $U(k)$.

Proof. We proceed our proof by estimating the roots of the characteristic polynomials of $S_3^1(k)$ and $S_4^1(k)$. Let x_1, x_2 ($x_1 > x_2$) be the two positive roots of $f(x) = x^4 - (k+4)x^2 - 2x + 1$ and y_1, y_2, y_3 ($y_1 > y_2 > y_3$) be the three roots of $g(y) = y^3 - (k+4)y^2 + 4ky - 6$. Noticing that $g(1) > 0$ and $g(4) = g(0) = -6$, we have $y_i > 0$ ($i = 1, 2, 3$).

Hence,

$$E(S_3^1) = 2(k-2) + 2(x_1 + x_2),$$
$$E(S_4^1) = 2(k-4) + 2(\sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}).$$

From our Appendix Table, it suffices to prove that $x_1 + x_2 + 2 > \sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}$ for $k \geq 50$. Consider the above function $f(x)$. Because $f(\sqrt{k+4}) < 0$ and $f(0) > 0$, we have $x_1 > \sqrt{k+4}$. Since $x_2 > 0$, we only need to show that

$$\sqrt{k+4} + 2 > \sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}. \tag{1}$$

Since $g(1) > 0$ and $g(4) = g(0) = -6$, we have $y_2 < 4$. Let $y = \frac{2}{k}$. Note that $g(\frac{2}{k}) = (\frac{2}{k})^3 - \frac{4}{k} - \frac{16}{k^2} + 8 - 6 > 0$ for $k \geq 50$, which means that $y_3 < \frac{2}{k}$. Hence, to finish the proof, it suffices to show that

$$\sqrt{y_1} < \sqrt{k+4} - \sqrt{\frac{2}{k}}. \tag{2}$$

At first, when $y = k + \frac{1}{2}$ and $k \geq 50$, we get that

$$g(k+\frac{1}{2}) = -\frac{7}{2}(k+\frac{1}{2})^2 + 4k(k+\frac{1}{2}) - 6 = (k+\frac{1}{2})(\frac{1}{2}k - \frac{7}{4}) - 6 > 0,$$

which implies that $y_1 < k + \frac{1}{2}$. Then, we only need to prove that

$$\sqrt{k+\frac{1}{2}} < \sqrt{k+4} - \sqrt{\frac{2}{k}}. \tag{3}$$

In fact, it is easy to check that $\frac{17}{4}k^2 - 18k + 4 > 0$ for $k \geq 50$, from which we have that $8k(k+\frac{1}{2}) < \frac{49}{4}k^2 - 14k + 4$. Then, we get that $2 + 2\sqrt{2}\sqrt{k(k+\frac{1}{2})} < \frac{7}{2}k$, which implies that $\sqrt{k(k+\frac{1}{2})} < \sqrt{k(k+4)} - \sqrt{2}$. By dividing $\sqrt{k}$ from the two sides of the last inequality, we get the required Inequality (3), and then the proof is complete. $\square$

Finally, we point out that the Appendix table of [2] has problems for the energies of $S_4^1(k)$ for almost all $k \leq 50$. We re-computed the energies of $S_4^1(k)$ and $S_3^1(k)$ for $5 \leq k \leq 100$. Our computation result is given in the following appendix table.

References

[1] I. Gutman, X. Li, J. Zhang, *Graph Energy*, in: M. Dehmer, F. Emmert-Streib (Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley-VCH Verlag, Weinheim, (2009) 145-174.

[2] X. Li, J. Zhang, B. Zhou, On unicyclic conjugated molecules with minimal energies, *J. Math. Chem.* **42** (2007) 729-740.

Appendix Table

$n = 2k$	$E(S_4^1(k))$	$E(S_3^1(k))$	$n = 2k$	$E(S_4^1(k))$	$E(S_3^1(k))$
$k = 5$	11.4006	12.0355	$k = 53$	116.8829	117.1020
$k = 6$	13.7663	14.3551	$k = 54$	119.0167	119.2338
$k = 7$	16.1047	16.6598	$k = 55$	121.1494	121.3645
$k = 8$	18.4251	18.9516	$k = 56$	123.2809	123.4941
$k = 9$	20.7301	21.2319	$k = 57$	125.4113	125.6226
$k = 10$	23.0219	23.5020	$k = 58$	127.5406	127.7501
$k = 11$	25.3019	25.7628	$k = 59$	129.6688	129.8765
$k = 12$	27.5715	28.0153	$k = 60$	131.7960	132.0019
$k = 13$	29.8318	30.2602	$k = 61$	133.9221	134.1264
$k = 14$	32.0837	32.4982	$k = 62$	136.0473	136.2499
$k = 15$	34.3279	34.7297	$k = 63$	138.1715	138.3725
$k = 16$	36.5652	36.9553	$k = 64$	140.2948	140.4942
$k = 17$	38.7960	39.1754	$k = 65$	142.4171	142.6150
$k = 18$	41.0209	41.3904	$k = 66$	144.5385	144.7349
$k = 19$	43.2403	43.6006	$k = 67$	146.6590	146.8540
$k = 20$	45.4545	45.8064	$k = 68$	148.7787	148.9722
$k = 21$	47.6641	48.0079	$k = 69$	150.8975	151.0896
$k = 22$	49.8691	50.2055	$k = 70$	153.0155	153.2062
$k = 23$	52.0700	52.3994	$k = 71$	155.1327	155.3220
$k = 24$	54.2669	54.5897	$k = 72$	157.2491	157.4371
$k = 25$	56.4602	56.7767	$k = 73$	159.3647	159.5514
$k = 26$	58.6499	58.9605	$k = 74$	161.4795	161.6650
$k = 27$	60.8362	61.1413	$k = 75$	163.5936	163.7778
$k = 28$	63.0194	63.3192	$k = 76$	165.7070	165.8899
$k = 29$	65.1996	65.4944	$k = 77$	167.8196	168.0014
$k = 30$	67.3770	67.6669	$k = 78$	169.9315	170.1121
$k = 31$	69.5516	69.8370	$k = 79$	172.0427	172.2222
$k = 32$	71.7236	72.0046	$k = 80$	174.1533	174.3316
$k = 33$	73.8931	74.1699	$k = 81$	176.2631	176.4404
$k = 34$	76.0603	76.3331	$k = 82$	178.3724	178.5485
$k = 35$	78.2251	78.4941	$k = 83$	180.4809	180.6560
$k = 36$	80.3878	80.6530	$k = 84$	182.5889	182.7629
$k = 37$	82.5483	82.8100	$k = 85$	184.6962	184.8691
$k = 38$	84.7068	84.9651	$k = 86$	186.8029	186.9748
$k = 39$	86.8634	87.1184	$k = 87$	188.9090	189.0799
$k = 40$	89.0180	89.2699	$k = 88$	191.0145	191.1845
$k = 41$	91.1709	91.4197	$k = 89$	193.1194	193.2884
$k = 42$	93.3219	93.5678	$k = 90$	195.2237	195.3918
$k = 43$	95.4713	95.7144	$k = 91$	197.3275	197.4947
$k = 44$	97.6191	97.8594	$k = 92$	199.4308	199.5970
$k = 45$	99.7652	100.0029	$k = 93$	201.5334	201.6988
$k = 46$	101.9099	102.1449	$k = 94$	203.6356	203.8000
$k = 47$	104.0530	104.2856	$k = 95$	205.7372	205.9008
$k = 48$	106.1947	106.4249	$k = 96$	207.8383	208.0010
$k = 49$	108.3350	108.5628	$k = 97$	209.9389	210.1007
$k = 50$	110.4739	110.6994	$k = 98$	212.0390	212.2000
$k = 51$	112.6115	112.8348	$k = 99$	214.1386	214.2987
$k = 52$	114.7478	114.9690	$k = 100$	216.2376	216.3970