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Solutions to Unsolved Problems on the Minimal Energies of Two Classes of Graphs

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Abstract

Let G be a graph and $\lambda_1, \lambda_2, \ldots \lambda_n$ be its eigenvalues. Then the energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots |\lambda_n|$. Let $\mathscr{B}(n)$ be the class of bipartite bicyclic graphs on n vertices containing a cycle with length congruent to 2 modulo 4. In [Z. Liu, B. Zhou, Minimal energies of bipartite bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 381–396] it was an attempted to determine the graph that has the minimal energy in $\mathscr{B}(n)$, but left two kinds of graphs B_n^1 and B_n^2 without determining which has the minimal energy. Let $\mathscr{G}_n$ be the class of tricyclic graphs G on n vertices that contain no disjoint odd cycles C_p, C_q of lengths p and q with $p + q \equiv 2 \pmod 4$. In [S. Li, X. Li, Z. Zhu, On tricyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem* **59** (2008) 397–419] it was attempted to characterize the minimal and second-minimal energies of graphs in $\mathscr{G}_n$, but left four kinds of graphs R_n, W_n, S_n, and Q_n without determining their ordering. This paper is to solve the two unsolved problems completely, and obtain that in $\mathscr{G}_n$, G_n^0, and G_n^1 have the minimal and second-minimal energy for $n \geq 10$, respectively, and in $\mathscr{B}_n$, B_n^1 has the minimal energy for $n \leq 31$, otherwise, B_n^2 for $n > 31$. The methods we use is different from those previously used. One is the approximate root method and the other is the well-known Coulson integral formula.

1 Preliminaries

In the paper, all the graphs under consideration are finite, connected and simple. We use P_n, C_n and S_n to denote the path, cycle and star with n vertices, respectively.

Let G be a graph of order n and $A(G)$ the adjacency matrix of G. The characteristic polynomial of G is

$$\phi(G,x) = det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i \lambda^{n-i} \ . \tag{1}$$

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\phi(G,\lambda) = 0$ are called the eigenvalues of G. Since $A(G)$ is symmetric, all the eigenvalues of G are real.

The energy of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=0}^{n} |\lambda_i|$. This graph–spectrum based invariant is much studied in mathematical chemistry; see the reviews [3, 4], the recent papers [7, 12, 14, 15, 20, 21] and the references cited therein. In particular, it is known [3, 5, 6] that $E(G)$ can be expressed by means of the Coulson integral formula

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[\left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i \, a_{2i} x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i \, a_{2i+1} x^{2i+1} \right)^2 \right] \mathrm{d}x \tag{2}$$

where $a_1, a_2, \ldots, a_n$ are the coefficients of the characteristic polynomial $\phi(G,x)$ of G. Let $b_{2i}(G) = (-1)^i \, a_{2i}(G)$ and $b_{2i+1}(G) = (-1)^i \, a_{2i+1}(G)$ for $0 \le i \le \lfloor \frac{n}{2} \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G. If $b_{2i}(G)$ (resp. $b_{2i+1}(G)$) assume nonnegative (resp., nonpositive) signs for $i = 0, 1, \ldots, n$, it follows from Eq.(2) that $E(G)$ is a monotonically increasing function in $b_i(G)$ for $i = 0, 1, \ldots, n$. That is, for any two graphs G_1 and G_2, we have

$$b_i(G_1) \ge b_i(G_2) \quad \text{for all}\, i \ge 0 \quad \Longrightarrow E(G_1) \ge E(G_2) \ .$$

If $b_i(G_1) \ge b_i(G_2)$ holds for all $i \ge 0$, then we denote $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$ (or $G_2 \preceq G_1$) and there is some i_0 satisfying $b_{i_0}(G_1) > b_{i_0}(G_2)$, then we denote $G_1 \succ G_2$ (or $G_2 \prec G_1$). Therefore, we have the following relation:

$$G_1 \succeq G_2 \Longrightarrow E(G_1) \ge E(G_2)$$

$$G_1 \succ G_2 \Longrightarrow E(G_1) > E(G_2) \ . \tag{3}$$

The above relation is just the quasi-order (i. e., "$\succ$") introduced in [6].

The following lemma is a well-known conclusion, known as the Coulson–Jacobs formula [2, 3, 19].

Lemma 1.1. *If G_1 and G_2 are two graph with the same number of vertices, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \frac{\phi(G_1; ix)}{\phi(G_2; ix)} \, \mathrm{d}x \ .$$

After these preparations, we will solve two unsolved problems on the minimal energies of two classes of graphs, left in [13, 18].

2 Solution to the unsolved problem in [13]

Since it is difficult to precisely calculate the non-zero eigenvalues of the characteristic polynomial of ascertained graphs for an arbitrary n, some scholars used to figure out energies of graphs and proceed effective comparison through estimating approximate roots of its eigenvalues, i. e., it is usually called the approximate root method.

Let $\mathscr{G}_n$ be the class of tricyclic graph G with n vertices that contain no disjoint two odd cycles C_p, C_q with $p+q \equiv 2 \pmod 4$. Denote G_n^0 as the graph obtained by connecting 3 pendent vertices to a vertex of degree 1 of the $K_{1,n-1}$, and G_n^1 as the graph formed by joining $n-6$ pendent vertices to a vertex of degree 4 of the complete bipartite graph $K_{2,4}$ (see Figure 1).

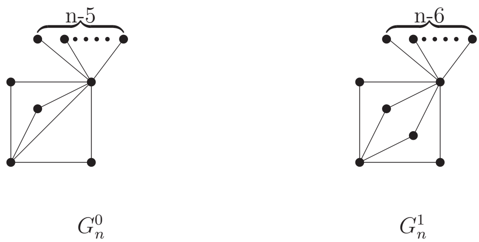

Fig.1. The graphs G_n^0 and G_n^1.

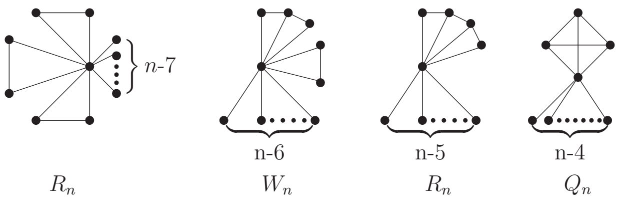

Fig.2. The graphs R_n , W_n , S_n , and G_n^1 .

In $\mathscr{G}_n$, there are four special graphs, which are named as R_n , W_n , S_n , and Q_n , respectively, where R_n has $n-7$ pendent vertices, W_n has $n-6$ pendent vertices, S_n has $n-5$ pendent vertices and Q_n has $n-4$ pendent vertices (see Figure 2).

Recently, Li et al.[13] wanted to determine the graphs having the minimal and second-minimal energies in $\mathscr{G}_n\,(n \geq 11)$. This conclusion is a partial proof of the case $e = n+2$ for $n \geq 7$ of a conjecture in [1], but has the constrained condition that it cannot contain the above four special graphs.

In this section we will show that the result is valid for all graphs in $\mathscr{G}_n$. In fact, the conclusion is also true for $n = 10$. Firstly, we restate the main result of [13] as follows.

Theorem 2.1. *(i) G_n^1 has the minimal energy in $\mathscr{G}_n$ for $7 \leq n \leq 10$;*
(ii) If $G \in \mathscr{G}_n$ and $G \notin \{R_n, W_n, S_n, Q_n, G_n^0, G_n^1\}$, then $E(G_n^0) < E(G_n^1) < E(G)$ for $n \geq 11$.

By simple calculation, we immediately have the following lemma.

Lemma 2.2.

$$
\begin{aligned}
\phi(Q_n;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} - 8\lambda^{n-3} + (3n-15)\lambda^{n-4} + (2n-8)\lambda^{n-5} \\
\phi(R_n;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} - 6\lambda^{n-3} + (3n-6)\lambda^{n-4} + 12\lambda^{n-5} - (3n-14)\lambda^{n-6} - 6\lambda^{n-7} \\
\phi(W_n;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} - 6\lambda^{n-3} + (3n-9)\lambda^{n-4} + 8\lambda^{n-5} - (2n-12)\lambda^{n-6} \\
\phi(S_n;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} - 6\lambda^{n-3} + (3n-12)\lambda^{n-4} + 2\lambda^{n-5} - (n-5)\lambda^{n-6} \\
\phi(G_n^0;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} - 6\lambda^{n-3} + (3n-15)\lambda^{n-4} \\
\phi(G_n^1;\lambda) &= \lambda^n - (n+2)\lambda^{n-2} + (4n-24)\lambda^{n-4}\ .
\end{aligned}
$$

Theorem 2.3. *For $n \geq 10$, if $G \in \mathscr{G}_n$ and $G \ncong G_n^0, G_n^1$, then $E(G_n^0) < E(G_n^1) < E(G)$.*

In order to obtain the above assertion, we, from Theorem 2.1, only need to show the following lemma.

Lemma 2.4. *If $G \cong R_n, W_n, S_n, Q_n$, then $E(G) > E(G_n^1)$ for $n \geq 10$.*

Proof. From Lemma 2.2 and the quasi-order (3), it is not difficult to check that $E(S_n) < E(W_n) < E(R_n)$. Next, we consider the problem of the difference between the energies of Q_n and S_n, as well as those of $Q_n$and G_n^1. Therefore, now we only need to show the following two claims in the sequel.

Claim1: $E(Q_n) < E(S_n)$, for $n \geq 7$.

From Lemma 2.2, we have

$$\begin{aligned}
\phi(Q_n;x) &= x^n - (n+2)x^{n-2} - 8x^{n-3} + (3n-15)x^{n-4} + (2n-8)x^{n-5} \\
&= x^{n-5}(x+1)^2(x^3 - 2x^2 - (n-1)x + (2n-8)) \\
&:= x^{n-5}(x+1)^2 f_1(x)
\end{aligned}$$

$$\begin{aligned}
\phi(S_n;x) &= x^{n-6}(x^6 - (n+2)x^4 - 6x^3 + (3n-12)x^2 + 2x - (n-5)) \\
&:= x^{n-6} f_2(x)\ .
\end{aligned}$$

It is easy to see that

$$\begin{aligned}
f_1(-\sqrt{n}) &= -\sqrt{n} - 8 < 0 && (n > 0) \\
f_1(-2) &= 4n - 26 > 0 && (n > 6) \\
f_1(2 - 7/n) &= \frac{n^3 - 35n^2 + 196n - 343}{n^3} > 0 && (n > 28) \\
f_1(2) &= -56 < 0 && (n > 0) \\
f_1(\sqrt{n-1}) &= -6 < 0 && (n > 0) \\
f_1(\sqrt{n}) &= \sqrt{n} - 8 \geq 0 && (n \geq 64)
\end{aligned}$$

According to the theorem of zeros of continued functions, we arrive at

$$2\left((2 - \frac{7}{n}) + \sqrt{n-1}\right) < E(Q_n) \quad \text{for } n > 28 \tag{4}$$

$$E(Q_n) < 2(2+\sqrt{n}) \qquad \text{for } n \geq 64\,. \tag{5}$$

It is also easy to see that

$$\begin{aligned}
f_2(-\sqrt{n}) &= n^2+6n^{\frac{3}{2}}-13n-2\sqrt{n}+5 > n^2-9n+5 > 0 & (n>9)\\
f_2(-2) &= -5n+33 < 0 & (n>6)\\
f_2(-1) &= n-4 > 0 & (n>4)\\
f_2(0) &= -(n-5) < 0 & (n>5)\\
f_2(0.6) &= -0.0496n+0.371456 > 0 & (n>7)\\
f_2(7/4) &= -\frac{206607}{4096}-\frac{305}{256}n < 0 & (n>0)\\
f_2(\sqrt{n-1}) &= -10n-6(n-1)\sqrt{n-1}+2\sqrt{n-1}+14 < 0 & (n>1)\\
f_2(\sqrt{n}) &= n^2-6n\sqrt{n}-13n+2\sqrt{n}+5 > 0 & (n>59)\ .
\end{aligned}$$

Again, according to the theorem of zeros of continued functions, we arrive at

$$2(0.6+1.75+\sqrt{n-1}) < E(S_n) \qquad \text{for } n > 7\,. \tag{6}$$

It follows from $\sqrt{n} < 0.35+\sqrt{n-1}$ with $n \geq 3$ that the right-hand side of (5) is less than the left-hand side of (6). Hence $E(Q_n) < E(S_n)$ for $n \geq 64$. Direct calculation yields that $E(Q_n) < E(S_n)$ for $7 \leq n \leq 63$, see Table 1.

Next, we will do the remaining part of the proof.

Claim 2: $E(G_n^1) < E(Q_n)$, for $n \geq 7$.

From Lemma 3.2, we have

$$\begin{aligned}
\phi(G_n^1;x) &= x^{n-4}(x^4-(n+2)x^2+(4n-24))\\
&\triangleq x^{n-4}f_3(x)\ .
\end{aligned}$$

Since

$$\begin{aligned}
f_3(1) &= 3n-25 > 0 & (n>8)\\
f_3(2-4/n) &= \frac{-112n^3+352n^2-512n+256}{n^4} < 0 & (n>3)\\
f_3(\sqrt{(n-7/4)}) &= \frac{n}{4}-\frac{279}{16} > 0 & (n>69)
\end{aligned}$$

therefore we have

$$E(G_n^1) < 2\left((2-\frac{4}{n})+\sqrt{(n-\frac{7}{4})}\right) \qquad \text{for } n > 69\,. \tag{7}$$

It follows from $3n^2 - 12n\sqrt{4n-7} - 36 > 0$ with $n > 62$ that the right–hand side of (7) is less than the left–hand side of (4). So $E(G_n^1) < E(Q_n)$ for $n > 69$. By straightforward computing, we also have that $E(G_n^1) < E(Q_n)$ for $7 < n \leq 69$, see Table 2.

It is easy to get that $E(G_{10}^1) > E(G_{10}^0)$ by direct calculation. Therefore, the proof is complete. □

Table1. The difference between $E(S_n)$ and $E(Q_n)$

n	$E(S_n) - E(Q_n)$	n	$E(S_n) - E(Q_n)$	n	$E(S_n) - E(Q_n)$
$n = 7$	0.33131	$n = 8$	0.26381	$n = 9$	0.28413
$n = 10$	0.39805	$n = 11$	0.41813	$n = 12$	0.41087
$n = 13$	0.42196	$n = 14$	0.42691	$n = 15$	0.43099
$n = 16$	0.43442	$n = 17$	0.43734	$n = 18$	0.43985
$n = 19$	0.44204	$n = 20$	0.43985	$n = 21$	0.44566
$n = 22$	0.44717	$n = 23$	0.44853	$n = 24$	0.44976
$n = 25$	0.45086	$n = 26$	0.45187	$n = 27$	0.45279
$n = 28$	0.45364	$n = 29$	0.45441	$n = 30$	0.45514
$n = 31$	0.45580	$n = 32$	0.45641	$n = 33$	0.45698
$n = 34$	0.45753	$n = 35$	0.45803	$n = 36$	0.45849
$n = 37$	0.45894	$n = 38$	0.45935	$n = 39$	0.45974
$n = 40$	0.46011	$n = 41$	0.46046	$n = 42$	0.46079
$n = 43$	0.46110	$n = 44$	0.46140	$n = 45$	0.46168
$n = 46$	0.46195	$n = 47$	0.46220	$n = 48$	0.46245
$n = 49$	0.46268	$n = 50$	0.46290	$n = 51$	0.4631
$n = 52$	0.46332	$n = 53$	0.46351	$n = 54$	0.46371
$n = 55$	0.46388	$n = 56$	0.46405	$n = 57$	0.46418
$n = 58$	0.46438	$n = 59$	0.46453	$n = 60$	0.46468
$n = 61$	0.46482	$n = 62$	0.46496	$n = 63$	0.46509

Table2. The difference between $E(Q_n)$ and $E(G_n^1)$

n	$E(Q_n)-E(G_n^1)$	n	$E(Q_n)-E(G_n^1)$	n	$E(Q_n)-E(G_n^1)$
$n=7$	1.05420	$n=8$	0.83081	$n=9$	0.70536
$n=10$	0.62183	$n=11$	0.55206	$n=12$	0.51447
$n=13$	0.47707	$n=14$	0.44648	$n=15$	0.42070
$n=16$	0.39865	$n=17$	0.37953	$n=18$	0.36275
$n=19$	0.34787	$n=20$	0.33457	$n=21$	0.32259
$n=22$	0.31172	$n=23$	0.30182	$n=24$	0.29273
$n=25$	0.28437	$n=26$	0.27665	$n=27$	0.26948
$n=28$	0.26280	$n=29$	0.25656	$n=30$	0.25072
$n=31$	0.24524	$n=32$	0.24006	$n=33$	0.23621
$n=34$	0.23160	$n=35$	0.22624	$n=36$	0.22220
$n=37$	0.21816	$n=39$	0.21442	$n=39$	0.21085
$n=40$	0.20744	$n=41$	0.20420	$n=42$	0.20107
$n=43$	0.19808	$n=44$	0.19521	$n=45$	0.19246
$n=46$	0.19080	$n=47$	0.18726	$n=48$	0.18420
$n=49$	0.18244	$n=50$	0.18015	$n=51$	0.17795
$n=52$	0.17782	$n=53$	0.17276	$n=54$	0.17186
$n=55$	0.16983	$n=56$	0.16796	$n=57$	0.16615
$n=58$	0.16439	$n=59$	0.16268	$n=60$	0.16102
$n=61$	0.15941	$n=62$	0.15785	$n=63$	0.15632
$n=64$	0.15483	$n=65$	0.15339	$n=66$	0.15198
$n=67$	0.15061	$n=68$	0.14927	$n=69$	0.14797

3 Solution to the unsolved problem in [18]

First we recall some notations. Let $\mathscr{B}(n)$ be the set of n-vertex bipartite graphs that contain a cycle of length $\equiv 2\,(\bmod 4)$. Let B be the graph with 6 vertices obtained by identifying an edge of two quadrangles. Denote by B_n^1 the graph formed by attaching $n-6$ pendent vertices to a vertex of degree 2 of B. By B_n^2 we denote the graph formed by attaching $n-6$ pendent vertices. Let B_n^3 be the graph obtained by identifying a vertex of a hexagon and a vertex of a quadrangle, and attaching $n-9$ pendent vertices to this common vertex. Let B_n^4 be the graph obtained by introducing an edge between a vertex of a hexagon and a vertex of a quadrangle, and attaching $n-10$ pendent vertices to the vertex of degree 3 in the hexagon. See Fig.3 for these graphs.

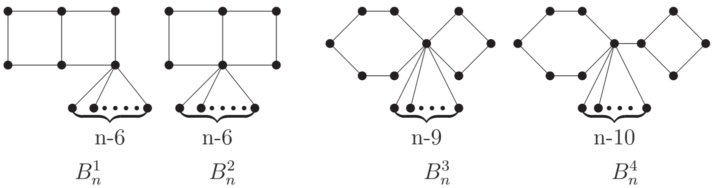

Fig.3. The graphsB_n^1 , B_n^2 , B_n^3 and B_n^4 .

Let $\mathscr{B}_1$,$\mathscr{B}_2$ and $\mathscr{B}_3$ be the class of graphs that contain three cycles, two cycles just having one common vertex and two vertex-disjoint cycles, respectively. Liu and Zhou [18] characterized the graph B_n^1 or B_n^2 , B_n^3 and B_n^4 have the minimal energy in the three classes $\mathscr{B}_1$,$\mathscr{B}_2$ and $\mathscr{B}_3$ of graphs, respectively. Furthermore, they almost completely obtained the graphs that have the minimal energy in $\mathscr{B}(n)$. Thus, which of the graphs B_n^1 and B_n^2 that has the minimal energy was not determined. In this section, we shall solve this unsolved problem and obtain that the graph B_n^1 and B_n^2 has the minimal and second-minimal energy in $\mathscr{B}(n)$ for $31 \geq n \geq 7$, respectively, and otherwise, B_n^2 and B_n^1 for $n > 31$.

Liu and Zhou [18] got the following result.

Theorem 3.1. *If $G \in \mathscr{B}(n)$ and $G \neq B_n^1, B_n^2$, where $n \geq 8$, then $E(G) > E(B_n^2)$.*

They also remarked that $E(B_n^1) < E(B_n^2)$ for $7 \leq n \leq 20$, but for $n \geq 7$ the common comparing way is invalid, since

$$b_2(B_n^1) = 5n - 23 > 4n - 17 = b_2(B_n^2), b_3(B_n^1) = 2n - 11 < 4n - 17 = b_3(B_n^2) \ . \qquad (8)$$

By simple calculation, their characteristic polynomials can be expressed as follows.

Lemma 3.2.

$$\begin{aligned}\phi(B_n^1;\lambda) &= \lambda^n-(n+1)\lambda^{n-2}+(5n-23)\lambda^{n-4}-(2n-11)\lambda^{n-6}\\ \phi(B_n^2;\lambda) &= \lambda^n-(n+1)\lambda^{n-2}+(4n-17)\lambda^{n-4}-(3n-17)\lambda^{n-6}\ .\end{aligned}$$

Before exhibiting our main result, we should prepare some knowledge on real analysis [23].

Lemma 3.3. *for any real number $X>-1$, we have*

$$\frac{X}{1+X}\le \log(1+X)\le X\ . \tag{9}$$

The following lemma[10, 11] will be very useful in the sequel.

Lemma 3.4. *Let A be a positive real number, B and C are non-negative. Then*

$$X=\frac{B-C}{A+C}>-1\ .$$

Now we will describe our main result in the section. That is, the graphs with the minimal and second-minimal energies in $\mathscr{B}(n)$ are uniquely ascertained.

Theorem 3.5. *If $G\in\mathscr{B}(n)$ and $G\ne B_n^1,B_n^2$, then*
(i) $E(B_n^1)<E(B_n^2)<E(G)$ for $7\le n\le 31$;
(ii) $E(B_n^2)<E(B_n^1)<E(G)$ for $n>31$.

Proof. Clearly, the common comparing method is failed for $E(B_n^1)$ and $E(B_n^2)$ by inequalities (8). That is, it can not be determined completely by just comparing the corresponding coefficients of their characteristic polynomials. But we can use the well-known Coulson integral formula to compare the energies of the two graphs completely. By Lemmas 1.1 and 3.2, we arrive at

$$E(B_n^1)-E(B_n^2)=\frac{1}{\pi}\int_{\infty}^{+\infty}\log\frac{x^6+(n+1)x^4+(5n-23)x^2+(2n-11)}{x^6+(n+1)x^4+(4n-17)x^2+(3n-17)}\,\mathrm{d}x\ . \tag{10}$$

Denote $f(x,n)$ as the integrand in Eq.(10). By letting $A=x^6+(n+1)x^4$, $B=(5n-23)x^2+(2n-11)$ and $C=(4n-17)x^2+(3n-17)$, $f(x,n)$ can be expressed as

$$f(x,n)=\log\frac{A+B}{A+C}=\log\left(1+\frac{B-C}{A+C}\right)$$

i. e.,

$$f(x,n)=\log\left(1+\frac{(n-6)(x^2-1)}{x^6+(n+1)x^4+(4n-17)x^2+(3n-17)}\right)$$

Obviously, $A>0$,$B\geq 0$ and $C\geq 0$ for $n\geq 6$. Now let $X=\frac{B-C}{A+C}$. Then by Lemmas 3.3 and 3.4, we obtain that for all $x\in\mathbb{R}$ and any integer $n\geq 6$,

$$f(x,n)\leq\frac{(n-6)(x^2-1)}{x^6+(n+1)x^4+(4n-17)x^2+(3n-17)}$$

and

$$f(x,n)\geq\frac{(n-6)(x^2-1)}{x^6+(n+1)x^4+(5n-23)x^2+(2n-11)}\ .$$

It follows that

$$f(x,n)\leq\frac{(n-6)(x^2-1)}{x^6+(n+1)x^4+(4n-17)x^2+(3n-17)}<0,\quad\text{if}\quad |x|<1 \tag{11}$$

and

$$f(x,n)\geq\frac{(n-6)(x^2-1)}{x^6+(n+1)x^4+(5n-23)x^2+(2n-11)}>0,\quad\text{if}\quad |x|>1\ . \tag{12}$$

Notice that the function sequence{f(x,n)} is convergent (if $x\neq 0$), and

$$\lim_{p\to+\infty}f(x,n)=\log\frac{x^4+5x^2+2}{x^4+4x^2+3}\ .$$

For convenience, let $\psi(x)=\log\frac{x^4+5x^2+2}{x^4+4x^2+3}$ be the limit of $\{f(x,n)\}$. For $x\neq 0$, we get

$$\begin{aligned}
&\psi(x)-f(x,n)\\
&=\log\frac{x^4+5x^2+2}{x^4+4x^2+3}-\log\frac{x^6+(n+1)x^4+(5n-23)x^2+(2n-11)}{x^6+(n+1)x^4+(4n-17)x^2+(3n-17)}\\
&=\log\frac{x^{10}+(n+6)x^8+(9n-10)x^6+(25n-100)x^4+(23n-119)x^2+(64n-34)}{x^{10}+(n+5)x^8+(9n-16)x^6+(25n-100)x^4+(23n-113)x^2+(64n-33)}
\end{aligned}$$

It is convenient to set

$$\mathbf{g_1(x)}=x^{10}+(n+6)x^8+(9n-10)x^6+(25n-100)x^4+(23n-119)x^2+(64n-34)$$

and

$$\mathbf{g_2(x)}=x^{10}+(n+5)x^8+(9n-16)x^6+(25n-100)x^4+(23n-113)x^2+(64n-33)\ .$$

Now let $A=x^{10}+(n+5)x^8+(9n-16)x^6+(25n-100)x^4+(23n-119)x^2+(64n-34)$, $B=x^8+6x^6$ and $C=6x^2+1$. Then $\psi(x)-f(x,n)$ can be translated into

$$\psi(x)-f(x,n)=\log\frac{A+B}{A+C}=\log\left(1+\frac{B-C}{A+C}\right)$$

i. e.,

$$\psi(x) - f(x,n) = \log\left(1 + \frac{x^8 + 6x^6 - 6x^2 - 1}{g_2(x)}\right) .$$

It is easy to get that $A > 0$, $B \geq 0$ and $C \geq 0$. By Lemmas 3.3 and 3.4, we have, for all $x \in \mathbb{R}$ and any integer $n \geq 5$,

$$\psi(x) - f(x,n) \leq \frac{x^8 + 6x^6 - 6x^2 - 1}{g_2(x)}$$

and

$$\psi(x) - f(x,n) \geq \frac{x^8 + 6x^6 - 6x^2 - 1}{g_1(x)} .$$

Since $B - C = x^8 + 6x^6 - 6x^2 - 1 = (x^2-1)(x^6 + 7x^4 + 7x^2 + 1)$, it follows that

$$\psi(x) < f(x,n) \quad \text{if } 0 < |x| < 1 \tag{13}$$

$$\psi(x) > f(x,n) \quad \text{if } |x| > 1 . \tag{14}$$

Analogously, for $x \neq 0$, we will consider

$$\begin{aligned} & f(x,n+1) - f(x,n) \\ = & \log \frac{x^6 + (n+2)x^4 + (5n-18)x^2 + (2n-9)}{x^6 + (n+2)x^4 + (4n-13)x^2 + (3n-14)} \\ & - \log \frac{x^6 + (n+1)x^4 + (5n-23)x^2 + (2n-11)}{x^6 + (n+1)x^4 + (4n-17)x^2 + (3n-17)} \\ = & \log \frac{x^{12} + (2n+3)x^{10} + (n^2+12n-33)x^8 + (9n^2-17n-78)x^6 +}{x^{12} + (2n+3)x^{10} + (n^2+12n-34)x^8 + (9n^2-17n-84)x^6 +} \\ & \frac{(25n^2-175n+263)x^4 + (23n^2-209n+459)x^2 + (6n^2-61n+153)}{(25n^2-175n+263)x^4 + (23n^2-209n+465)x^2 + (6n^2-61n+154)} . \end{aligned}$$

It is also convenient to set $\mathbf{h_1(x)} = x^{12} + (2n+3)x^{10} + (n^2+12n-33)x^8 + (9n^2 - 17n - 78)x^6 + (25n^2 - 175n + 263)x^4 + (23n^2 - 209n + 459)x^2 + (6n^2 - 61n + 153)$ and $\mathbf{h_2(x)} = x^{12} + (2n+3)x^{10} + (n^2+12n-34)x^8 + (9n^2-17n-84)x^6 + (25n^2-175n+263)x^4 + (23n^2-209n+465)x^2 + (6n^2-61n+154)$. Now let $A = x^{12} + (2n+3)x^{10} + (n^2+12n-34)x^8 + (9n^2-17n-84)x^6 + (25n^2-175n+263)x^4 + (23n^2-209n+459)x^2 + (6n^2-61n+153)$, $B = x^8 + 6x^6$ and $C = 6x^2 + 1$. Then the above $f(x,n+1) - f(x,n)$ can be translated into

$$f(x,n+1) - f(x,n) = \log \frac{A+B}{A+C} = \log\left(1 + \frac{B-C}{A+C}\right)$$

i. e.,

$$f(x,n+1)-f(x,n)=\log\left(1+\frac{x^8+6x^6-6x^2-1}{h_2(x)}\right) .$$

Similarly, we have

$$f(x,n+1)-f(x,n)\leq\frac{x^8+6x^6-6x^2-1}{h_2(x)}$$

and

$$f(x,n+1)-f(x,n)\geq\frac{x^8+6x^6-6x^2-1}{h_1(x)} .$$

Because $B-C=x^8+6x^6-6x^2-1=(x^2-1)(x^6+7x^4+7x^2+1)$, it follows that

$$f(x,n+1)<f(x,n)<0 \quad \text{if } 0<|x|<1 \tag{15}$$

and

$$f(x,n+1)>f(x,n)>0 \quad \text{if } |x|>1\,. \tag{16}$$

Combining inequalities (11) through (16), we can deduce that

$$\psi(x)<f(x,n+1)<f(x,n) \quad \text{if } 0<|x|<1 \tag{17}$$

and

$$\psi(x)>f(x,n+1)>f(x,n) \qquad\qquad \text{if } |x|>1\,. \tag{18}$$

Together with inequalities (17) and (18), for $n>36$ it is straightforward to obtain that

$$\int\limits_0^{+\infty} f(x,n)\,\mathrm{d}x=\int\limits_0^{1} f(x,n)\,\mathrm{d}x+\int\limits_1^{+\infty} f(x,n)\,\mathrm{d}x>\int\limits_0^{1} \psi(x,n)\,\mathrm{d}x+\int\limits_1^{+\infty} f(x,36)\,\mathrm{d}x\,. \tag{19}$$

With computer-aided calculations and Lemma 3.3, for any $x>1$ we have

$$\begin{aligned} f(x,36) &= \log\frac{x^6+37x^4+157x^2+61}{x^6+37x^4+127x^2+91} \\ &= \log\left(1+\frac{30(x^2-1)}{x^6+37x^4+157x^2+61}\right) \\ &\geq \frac{30(x^2-1)}{x^6+37x^4+157x^2+61} \\ &\geq \frac{30(x^2-1)}{x^6+37.13x^4+157.901x^2+61.1116}\,. \end{aligned}$$

Moreover, we get

$$\begin{aligned}
\int_1^{+\infty} f(x,36)\mathrm{d}x &\geq \int_1^{+\infty} \frac{30(x^2-1)}{x^6+37x^4+157x^2+61}\,\mathrm{d}x \\
&\geq \int_1^{+\infty} \frac{30(x^2-1)}{x^6+37.13x^4+157.901x^2+61.1116}\,\mathrm{d}x \\
&= \int_1^{+\infty} \frac{30(x^2-1)}{(x^2+\frac{323}{10})(x^2+\frac{22}{5})(x^2+\frac{43}{100})}\,\mathrm{d}x \\
&= \frac{111000}{31911431}\sqrt{3230}\arctan\frac{\sqrt{3230}}{323} + \frac{4290000}{5440527}\sqrt{43}\arctan\frac{10}{43}\sqrt{43} \\
&\quad + \frac{4500}{135377}\sqrt{110}\pi - \frac{9000}{135377}\sqrt{110}\arctan\frac{\sqrt{110}}{22} - \frac{555000}{31911431}\sqrt{3230}\pi \\
&\quad - \frac{2145000}{54405277}\sqrt{43}\pi \\
&= 0.2088648803\ .
\end{aligned} \tag{20}$$

Table3. The difference between $E(B_n^1)$ and $E(B_n^2)$

n	$E(B_n^2)-E(B_n^1)$	n	$E(B_n^2)-E(B_n^1)$	n	$E(B_n^2)-E(B_n^1)$
$n=7$	0.06301	$n=17$	0.03370	$n=26$	0.00963
$n=8$	0.06812	$n=18$	0.02952	$n=27$	0.00779
$n=9$	0.06568	$n=19$	0.02653	$n=28$	0.00529
$n=10$	0.06141	$n=20$	0.02372	$n=29$	0.00415
$n=11$	0.05676	$n=20$	0.02372	$n=30$	0.00274
$n=12$	0.05214	$n=21$	0.02106	$\mathbf{n=31}$	**0.00081**
$n=13$	0.04875	$n=22$	0.01855	$\mathbf{n=32}$	**-0.00076**
$n=14$	0.04361	$n=23$	0.01617	$n=33$	-0.00228
$n=15$	0.03973	$n=24$	0.01392	$n=34$	-0.00373
$n=16$	0.03610	$n=25$	0.01177	$n=35$	-0.00513
				$n=36$	-0.00779

Meanwhile,

$$\begin{aligned}\int_0^1 \psi(x)\mathrm{d}x &= \int_0^1 \frac{x^4+5x^2+2}{x^4+4x^2+3}\,\mathrm{d}x \\ &= \frac{1}{192}\Bigg((60-12\sqrt{17})\arctan(\frac{2}{\sqrt{10-2\sqrt{17}}})\sqrt{10+2\sqrt{17}}-(96+64\sqrt{3})\pi \\ &+\ (60+12\sqrt{17})\arctan(\frac{2}{\sqrt{10+2\sqrt{17}}})\sqrt{10-2\sqrt{17}}\Bigg) \\ &= -0.2084288229\ . \end{aligned} \tag{21}$$

Consequently, associating Eqs.(19) through (21), the difference between the energies of B_n^1 and B_n^2 for $n \geq 36$ is determined by a positive number. Together with Table 3 , we surely complete the proof of the conclusion. □

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