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Energy Bounds for Graphs with Fixed Cyclomatic Number

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Abstract

We show that the maximum value of the graph energy within the set of all graphs with cyclomatic number k (which includes, for instance, trees or unicyclic graphs as special cases) is at most $4n/\pi + A_k$ for a constant A_k that only depends on k, and we show how to construct graphs of arbitrary cyclomatic number whose energy is indeed essentially $4n/\pi$. Similar results are also given for the minimum energy and for the Merrifield-Simmons index and the Hosoya index, two related graph parameters.

1 Introduction

The energy $\mathrm{En}(G)$ of a graph G, defined as the sum of the absolute values of the eigenvalues of a graph, is a popular graph invariant in mathematical chemistry, see for instance [5] for a recent survey. In the recent past, the general problem of determining the maximum or minimum value of the graph energy within a certain class of graphs has gained considerable interest. Results of this form are known for trees [4, 6, 11, 12, 17], unicyclic graphs [1, 8–10, 14], bicyclic graphs [7, 15, 19], tricyclic graphs [13], and so on. In this paper, we will generally consider connected graphs with fixed cyclomatic number k (i.e.,

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if the number of vertices is n, then the number of edges is $n + k - 1$), generalising the aforementioned classes (trees, for instance, correspond to the case $k = 0$).

While it becomes increasingly difficult to determine the exact maxima and minima of the energy and the associated graphs (for which these extremal values are attained) as k grows, we will see that one can at least give a qualitative answer to the general question what the maximum/minimum energy is, given k and the number of vertices n. It is known that the energy of a graph with m edges is at most $2m$ [2], so the growth can at most be linear if the cyclomatic number is fixed. As we will see, the constant 2 can essentially be replaced by $4/\pi$. The following theorem is the main result of this paper:

Theorem 1 *Let k be a fixed nonnegative integer, and denote the set of all connected graphs with n vertices and cyclomatic number k by $\mathcal{G}_{n,k}$. There exists a constant A_k depending only on k such that the inequality*

$$\frac{4n}{\pi} + A_k \geq \mathrm{En}(G)$$

holds for all $G \in \mathcal{G}_{n,k}$.

Moreover, it is not hard to construct graphs $H_n \in \mathcal{G}_{n,k}$ such that

$$\mathrm{En}(H_n) \geq \frac{4n}{\pi} + a_k$$

for some constant a_k. This is done in Section 4. It follows that

Corollary 2 *The maximum energy of a graph in $\mathcal{G}_{n,k}$ is $4n/\pi + O(1)$.*

Here and in the following, $O(1)$ terms refer to the situation that $n \to \infty$ while k is fixed. For the minimum, things are somewhat simpler: it is known that the energy of a graph without isolated vertices is at least $2\sqrt{n-1}$, with equality for the star [2]. In particular, the star has minimum energy among connected graphs. Moreover, it is well known [2] that $\mathrm{En}(G) \geq 2\sqrt{m}$ for all graphs G with m vertices, and so $\mathrm{En}(G) \geq 2\sqrt{n+k-1}$ for all graphs $G \in \mathcal{G}_{n,k}$. For the sake of completeness, we show in Section 4 how to construct graphs of arbitrary cyclomatic number whose energy is close to $2\sqrt{n}$. Hence we have:

Theorem 3 *The minimum energy of a graph in $\mathcal{G}_{n,k}$ is $2\sqrt{n} + O(1)$.*

This also implies that the limits

$$M_k = \limsup_{n\to\infty} \left(\max_{G\in G_{n,k}} \mathrm{En}(G) - \frac{4n}{\pi} \right)$$

and

$$m_k = \liminf_{n\to\infty} \left(\min_{G\in G_{n,k}} \mathrm{En}(G) - 2\sqrt{n} \right)$$

exist for all k. Not many explicit values of these limits are known, especially for the maximum. It is well known that the maximum energy of a tree is obtained for the path, and that this energy is

$$\mathrm{En}(P_n) = \begin{cases} 2\left(\csc(\pi/(2n+2)) - 1\right) & n \text{ even}, \\ 2\left(\cot(\pi/(2n+2)) - 1\right) & n \text{ odd}, \end{cases} \tag{1}$$

which proves that $M_0 = 4/\pi - 2 \approx -0.72676$. It is already considerably more effort to determine the constant in the case of unicyclic graphs: in [1], the value is found to be $M_1 \approx 0.11811$.

The key to our main theorem is, as in most results on the energy, the Coulson integral formula [4], which we use in the following form:

$$\mathrm{En}(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \left| x^n \phi(G, i/x) \right|, \tag{2}$$

where n is the order of G and $\phi(G, u)$ denotes the characteristic polynomial of G. Before we prove the main theorem, we consider two closely related graph invariants: the Merrifield-Simmons index and the Hosoya index. For these two invariants, the proof is much simpler, but they give a flavour of the type of argument that is used to obtain the main theorem.

2 Merrifield-Simmons index and Hosoya index

Recall that the Merrifield-Simmons index $\sigma(G)$ of a graph G is defined as the total number of independent sets, and the Hosoya index $z(G)$ is the total number of matchings of G. We prove inequalities analogous to those in Theorem 1 for the logarithm of $\sigma(G)$ and $z(G)$. The minimum of the Merrifield-Simmons index is known to occur typically for the same graphs within a fixed class as the maximum of the Hosoya index and the energy, see [18] for a survey of results along these lines.

The minimum of $z(G)$ and the maximum of $\sigma(G)$ are typically attained for "star-like graphs". Indeed, it was shown in [16, 20] that among graphs of order n with cyclomatic number $0 \leq k \leq n-2$, the graph with maximum Merrifield-Simmons index and minimum Hosoya index consists of k triangles sharing a common edge, and $n-k-2$ pendant vertices attached to one of the ends of this common edge (in two exceptional cases, there is a second graph with the same property). It is easy to see that this graph has Hosoya index $(k+1)n-2k$ and Merrifield-Simmons index $2^{n-2}+2^{n-k-2}+1$. From these two formulas, we can deduce:

Theorem 4 *The minimum of* $\log z(G)$ *for a graph* $G \in \mathcal{G}_{n,k}$ *is* $\log n + O(1)$*, the maximum of* $\log \sigma(G)$ *is* $n \log 2 + O(1)$*.*

Let generally H be any fixed graph and v a vertex of H, and define $S(\ell)$ as the graph that results by attaching ℓ pendant vertices to v. Then

$$\sigma(S(\ell)) = 2^{\ell}\sigma(H \setminus v) + \sigma(H \setminus N[v]),$$

where $N[v]$ is the closed neighbourhood of v (consisting of all neighbours of v and v itself). Likewise,

$$z(S(\ell)) = \ell z(H \setminus v) + z(H).$$

It follows that the graphs $S(\ell)$ so constructed are "almost optimal" in the sense that

$$\log \sigma(S(\ell)) = |S(\ell)| \log 2 + O(1) \tag{3}$$

and

$$\log z(S(\ell)) = \log |S(\ell)| + O(1). \tag{4}$$

Things are more complicated for the minimum of $\sigma(G)$ and the maximum of $z(G)$, and a similarly simple description of the extremal graphs does not seem to be possible. However, analogous estimates hold.

Let us consider the Merrifield-Simmons index first. We prove by induction on k that a graph $G \in \mathcal{G}_{n,k}$ satisfies

$$\sigma(G) \geq (3/4)^k F_{n+2},$$

where F_{n+2} denotes the $(n+2)$th Fibonacci number ($F_0 = 0$, $F_1 = 1$, $F_{n+1} = F_n + F_{n-1}$). For $k = 0$, we know that the path P_n has minimal Merrifield-Simmons index, and $\sigma(P_n) = F_{n+2}$. If now $G \in \mathcal{G}_{n,k+1}$, then we find an edge $e = uv$ in G that is contained in a cycle.

This edge reduces the number of independent sets by all those which contain both u and v. However, given any such independent set in $G \setminus e$, we can remove either u or v or both to obtain another independent set, which implies that at most $1/4$ of all independent sets of $G \setminus e$ contain u and v. It follows that

$$\sigma(G) \geq \frac{3}{4}\sigma(G \setminus e),$$

which completes the induction. An immediate consequence is that

$$\log \sigma(G) \geq n \log \frac{\sqrt{5}+1}{2} + O(1) \tag{5}$$

for $G \in \mathcal{G}_{n,k}$.

For the Hosoya index, consider a graph $G \in \mathcal{G}_{n,k}$, and take a spanning tree T of G. Let R be the set of the k remaining edges. Then any matching of G consists of a matching of T and a subset of the remaining k edges. It is well known that the maximum of $z(T)$ for a tree (or indeed any forest) T of order n is the Fibonacci number F_{n+1}, and there are 2^k subsets of the remaining edges. Hence

$$z(G) \leq 2^k F_{n+1}.$$

One can improve quite easily on this inequality: consider those matchings which induce a matching of cardinality r on R. When we remove the vertices incident with these r edges as well as all the other edges in R, we are left with a forest of order $n-2r$, which means that it has at most F_{n-2r+1} matchings. This shows that

$$z(G) \leq \sum_{r=0}^{k} \binom{k}{r} F_{n-2r+1} = \begin{cases} 5^{k/2} F_{n-k+1} & k \text{ even}\,, \\ 5^{(k-1)/2} L_{n-k+1} & k \text{ odd}\,. \end{cases}$$

Here, L_n denotes the Lucas numbers ($L_0 = 2$, $L_1 = 1$, $L_{n+1} = L_n + L_{n-1}$). It follows immediately that

$$\log z(G) \leq n \log \frac{1+\sqrt{5}}{2} + O(1)\,. \tag{6}$$

The inequalities (5) and (6) are sharp up to the $O(1)$-term. To see this, we construct graphs for which the values of σ and z are $n \log \frac{1+\sqrt{5}}{2} + O(1)$. Let again H be an arbitrary graph with a fixed vertex v, and define $P(\ell)$ to be the graph obtained by identifying one end of a path of length ℓ with v.

Then we have

$$\sigma(P(\ell)) = \sigma(P(\ell-1)) + \sigma(P(\ell-2)),$$

which shows that

$$\sigma(P(\ell)) = \beta_1 \left(\frac{1+\sqrt{5}}{2}\right)^n + \beta_1 \left(\frac{1-\sqrt{5}}{2}\right)^n$$

for certain constants β_1 (necessarily positive) and β_2. Taking the logarithm, we immediately get

$$\log \sigma(P(\ell)) = n \log \frac{1+\sqrt{5}}{2} + O(1).$$

The same can be done with the Hosoya index: the recursion

$$z(P(\ell)) = z(P(\ell-1)) + z(P(\ell-2))$$

holds, and we conclude

$$\log z(P(\ell)) = n \log \frac{1+\sqrt{5}}{2} + O(1)$$

as before. Combining the results, we found that

Theorem 5 *The maximum of* $\log z(G)$ *for a graph* $G \in \mathcal{G}_{n,k}$ *is* $n \log \frac{1+\sqrt{5}}{2} + O(1)$, *and the minimum of* $\log \sigma(G)$ *is* $n \log \frac{1+\sqrt{5}}{2} + O(1)$.

3 Proof of the main result

As mentioned in the introduction, we use the Coulson integral formula (2). By the celebrated Sachs theorem [3, Theorem 2.3.3], the characteristic polynomial $\phi(G, x)$ of a graph G of order n can be written as

$$\phi(G, x) = \sum_{k=0}^{n} c_k x^{n-k},$$

where

$$c_k = \sum_{H \in \mathcal{H}_k} (-1)^{p(H)} 2^{c(H)}.$$

Here, $\mathcal{H}_k$ stands for the set of all elementary subgraphs (graphs whose components are only single edges and cycles) of G with exactly k vertices, $p(H)$ is the number of components of H and $c(H)$ is the number of cycles of H. In (2), x is replaced by i/x, so we will mostly deal with

$$x^n \phi(G, i/x) = \sum_{k=0}^{n} i^{n-k} c_k x^k.$$

The triangle inequality yields

$$\left| x^n \phi(G, i/x) \right| \leq \sum_{k=0}^{n} \sum_{H \in \mathcal{H}_k} 2^{c(H)} x^k$$

for all $x \geq 0$, and equality holds in particular for trees. In the following, we denote the right hand side by $\psi(G,x)$, i.e.,

$$\left| x^n \phi(G, i/x) \right| \leq \psi(G,x). \tag{7}$$

It is obvious that $\psi(G \cup H, x) = \psi(G,x)\psi(H,x)$ (just like $\phi(G \cup H, x) = \phi(G,x)\phi(H,x)$, since elementary subgraphs of $G \cup H$ are unions of elementary subgraphs of G and H). Moreover, $\psi(G,x) \leq \psi(G',x)$ for all $x \geq 0$ if G is a subgraph of G'. In particular, the following simple inequality for paths that we will need later holds:

$$\psi(P_n,x) \geq \psi(P_2,x)\psi(P_{n-2},x) = (1+x^2)\psi(P_{n-2},x) \geq x^2\psi(P_{n-2},x). \tag{8}$$

Let us now review the following facts about trees:

Lemma 6 *1. If T is a tree of order n, then its characteristic polynomial is given by*

$$\phi(T,x) = \sum_{k \geq 0} (-1)^k m(T,k) x^{n-2k},$$

where $m(T,k)$ is the number of matchings of T consisting of exactly k edges, and

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

2. Among all trees of order n, the path P_n has the greatest number of matchings of any cardinality.

Proof: The formula for $\psi(T,x)$ follows (just like the formula for $\phi(T,x)$) from the fact that the only elementary subgraphs of trees are matchings. All other parts of the lemma are well known [4,5]. ■

The final ingredient to the proof of our main theorem is the following essential recursion:

Lemma 7 *Let $e = uv$ be an edge of the graph G. Then the recursion*

$$\phi(G,x) = \phi(G \setminus e, x) - \phi(G \setminus \{u,v\}, x) - 2 \sum_{Z \in \mathcal{C}(e)} \phi(G \setminus Z, x)$$

holds, where $\mathcal{C}(e)$ denotes the set of all cycles that contain e. Analogously,

$$\psi(G,x) = \psi(G \setminus e, x) + x^2 \psi(G \setminus \{u,v\}, x) + 2 \sum_{Z \in \mathcal{C}(e)} x^{|Z|} \psi(G \setminus Z, x).$$

Proof: The proof of the first part is classical, see [3, Theorem 2.3.4]. It is based on a one-to-one correspondence between elementary subgraphs of G and elementary subgraphs contributing to the right hand side. The proof of the second part follows along the same lines. ■

Now we are ready to prove the following crucial lemma, from which the main result will follow immediately:

Lemma 8 *There exist positive constants α_j, β_j for $j = 1, 2, \dots$ such that for any $G \in \mathcal{G}_{n,k}$ and any $x \geq 0$, the inequality*

$$\psi(G, x) \leq \prod_{j=1}^{k}(1 + \alpha_j x^2 + \beta_j x^3)\psi(P_n, x)$$

holds.

Proof: By induction on k. For $k = 0$, the statement is trivial by Lemma 6. Otherwise, let $e = uv$ be an edge of G that is contained in at least one cycle. Clearly, $G \setminus e \in \mathcal{G}_{n,k-1}$. Moreover, $G' = G \setminus \{u, v\}$ is a subgraph of a graph in $\mathcal{G}_{n-2,\ell}$ for some $\ell < k$: if it has r components, then each of them has an edge connecting it to either u or v in G, and at least one of the components has more than one such edge (any component that contains the rest of a cycle to which e belongs in G). Hence at least $r + 2$ edges were removed along with u and v. If we add $r - 1$ edges to G' to connect the components, then we obtain a connected graph with at least three edges less than G, but only two vertices less. So the cyclomatic number of this graph must be less than k, as claimed.

Similarly, $G \setminus Z$ is a subgraph of a graph in $\mathcal{G}_{n-|Z|,h(Z)}$ for any $Z \in \mathcal{C}(e)$, where $h(Z) < k$ (and clearly $|Z| \geq 3$). Now we can apply the induction hypothesis together with the recursion in Lemma 7 and the simple inequality (8) to obtain

$$\begin{aligned}
\psi(G, x) &= \psi(G \setminus e, x) + x^2\psi(G \setminus \{u, v\}, x) + 2\sum_{Z \in \mathcal{C}(e)} x^{|Z|}\psi(G \setminus Z, x) \\
&\leq \prod_{j=1}^{k-1}(1 + \alpha_j x^2 + \beta_j x^3)\left(\psi(P_n, x) + x^2\psi(P_{n-2}, x) + 2\sum_{Z \in \mathcal{C}(e)} x^{|Z|}\psi(P_{n-|Z|}, x)\right) \\
&\leq \prod_{j=1}^{k-1}(1 + \alpha_j x^2 + \beta_j x^3)\left(\psi(P_n, x) + x^2\psi(P_{n-2}, x) + 2\sum_{Z \in \mathcal{C}(e)} x^{2+\epsilon(Z)}\psi(P_{n-2-\epsilon(Z)}, x)\right),
\end{aligned}$$

where $\epsilon(Z)$ is 0 if Z has even length and 1 otherwise. The last step follows by repeatedly applying (8). Moreover, we have $\psi(P_{n-3}, x) \leq \psi(P_{n-2}, x) \leq \psi(P_n, x)$ and thus

$$\psi(G, x) \leq \prod_{j=1}^{k-1}(1 + \alpha_j x^2 + \beta_j x^3) \left(1 + x^2 + 2 \sum_{Z \in \mathcal{C}(e)} x^{2+\epsilon(Z)}\right) \psi(P_n, x).$$

Let us finally estimate the size of $\mathcal{C}(e)$: since we know that G has cyclomatic number k, $\mathcal{C}(e)$ contains less than 2^k elements (since the entire cycle space consists of 2^k elements, and the empty set is one of the elements of the cycle space). Therefore, we get

$$\psi(G, x) \leq \prod_{j=1}^{k}(1 + \alpha_j x^2 + \beta_j x^3)\psi(P_n, x)$$

with $\alpha_k = \beta_k = 2^{k+1}$, which completes the induction. ■

Proof of Theorem 1: Let G be any graph with n vertices and cyclomatic number k. The Coulson integral formula (2) together with the inequality (7) yields

$$\mathrm{En}(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \left| x^n \phi(G, i/x) \right| \leq \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \psi(G, x) \; .$$

Now apply the previous lemma to get

$$\mathrm{En}(G) \leq \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \psi(P_n, x) + \sum_{j=1}^{k} \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log(1 + \alpha_j x^2 + \beta_j x^3) \; .$$

As mentioned before, $\psi(P_n, x) = |x^n \phi(P_n, i/x)|$ since P_n is a tree. Therefore, the first integral is just $\mathrm{En}(P_n)$, which is $\leq 4n/\pi$, as can be seen from (1). The sum of the other integrals is a constant (note that all the integrals converge) that only depends on k, but not on n. This proves our theorem. ■

Remark 1 The constant A_k obtained from the proof is certainly not best possible and could be improved by estimating more carefully, but since the main point of the theorem is the existence of such constants, it seemed sensible to keep things as simple as possible. An explicit bound can be obtained as follows: by the change of variables $x = 2^{-j/2}u$, we get

$$\begin{aligned} \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log(1 + \alpha_j x^2 + \beta_j x^3) &= \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log(1 + 2^{j+1}x^2 + 2^{j+1}x^3) \\ &= 2^{j/2} \cdot \frac{2}{\pi} \int_0^\infty \frac{du}{u^2} \log(1 + 2u^2 + 2^{1-j/2}u^3) \end{aligned}$$

$$\leq 2^{j/2} \cdot \frac{2}{\pi} \int_0^\infty \frac{du}{u^2} \log(1 + 2u^2 + \sqrt{2}u^3)$$

$$< 3.75 \cdot 2^{j/2}$$

and thus

$$\sum_{j=1}^{k} \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log(1 + \alpha_j x^2 + \beta_j x^3) < 3.75 \cdot \sum_{j=1}^{k} 2^{j/2} < 13 \cdot 2^{k/2} \ .$$

4 Constructing graphs with large and small energy

It is not very hard to construct graphs with cyclomatic number k whose energy is $\sqrt{2n} + O(1)$ and $4n/\pi + O(1)$ respectively. Indeed, the simple idea is again to consider graphs that are "star-like" or "path-like". Let us first illustrate this for the simpler case of graphs with small energy and then consider graphs with large energy.

Let H be any fixed graph and v a vertex of H. Define $S(\ell)$ as in Section 2 as the graph that results by attaching ℓ pendant vertices to v. Then Lemma 7 yields

$$\phi(S(\ell), x) = x\phi(S(\ell-1), x) - x^{\ell-1} \cdot \phi(H \setminus v, x)$$

and by iteration

$$\phi(S(\ell), x) = x^\ell \phi(H, x) - \ell x^{\ell-1} \phi(H \setminus v, x) \ .$$

Now we obtain, with $n = |S(\ell)| = |H| + \ell$,

$$\begin{aligned} |x^n \phi(S(\ell), i/x)| &= \left| x^{|H|} \phi(H, i/x) + \ell i x^{|H|+1} \phi(H \setminus v, i/x) \right| \\ &= \left| x^{|H|} \phi(H, i/x) \right| \cdot \left| 1 + \ell i x \cdot \frac{\phi(H \setminus v, i/x)}{\phi(H, i/x)} \right| \\ &= \left| x^{|H|} \phi(H, i/x) \right| \cdot \left| 1 + \ell x^2 h(x) \right| \end{aligned}$$

for a rational function $h(x) = (i\phi(H \setminus v, i/x))/(x\phi(H, i/x))$ with the following properties:

- $h(x) = 1 + O(x^2)$ as $x \to 0$, which follows from the fact that the polynomials $\phi(H, i/x)$ and $\phi(H \setminus v, i/x)$ are of the form $(i/x)^H + a(i/x)^{H-2} + \cdots$ and $(i/x)^{H-1} + b(i/x)^{H-3} + \cdots$ respectively.

- $h(x) = O(x^r)$ for some integer r as $r \to \infty$ (which simply holds since $h(x)$ is a rational function without real poles).

We use these two facts to estimate the energy of $S(\ell)$, which is given by

$$\begin{aligned}
\mathrm{En}(S(\ell)) &= \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|x^n\phi(S(\ell),i/x)\right| \\
&= \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|x^{|H|}\phi(H,i/x)\right| + \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log(1+\ell x^2) \\
&+ \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|\frac{1+\ell x^2 h(x)}{1+\ell x^2}\right| \\
&= \mathrm{En}(H) + 2\sqrt{\ell} + \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|\frac{1+\ell x^2 h(x)}{1+\ell x^2}\right| .
\end{aligned}$$

As $\ell \to \infty$, the integrand in the last term converges to $x^{-2}\log|h(x)|$. To show that interchanging the limit and the integral is indeed possible, note first that $(1+\ell x^2 h(x))/(1+\ell x^2)$ is $1+O(x^2)$ uniformly in ℓ in an interval around 0 by the above properties of $h(x)$. Hence we can use uniform convergence within such an interval. For the remaining part of the integral, note first that both real and imaginary part of $h(x)$ are rational functions in x. If the imaginary part is not identically zero, we immediately get upper and lower bounds for $\left|\frac{1+\ell x^2 h(x)}{1+\ell x^2}\right|$ valid uniformly in ℓ, and these bounds are again rational functions. We can then use the dominated convergence theorem.

If the imaginary part is identically zero, then $h(x)$ is a strictly positive rational function, since the zeros of $\phi(H,i/x)$ and $\phi(H\setminus v,i/x)$ are purely imaginary, and they must be symmetric with respect to zero so that the imaginary part cancels. This, however, implies that numerator and denominator of $h(x)$ can be factored into terms of the form $1+ax^2$, proving positivity. Now we can again bound $\left|\frac{1+\ell x^2 h(x)}{1+\ell x^2}\right|$ above and below by rational functions uniformly in ℓ and apply the dominated convergence theorem.

So we finally get

$$\begin{aligned}
\lim_{\ell\to\infty}\left(\mathrm{En}(S(\ell)) - 2\sqrt{\ell}\right) &= \mathrm{En}(H) + \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log h(x) \\
&= \mathrm{En}(H) + \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|x^{|H|-1}\phi(H\setminus v,i/x)\right| \\
&- \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|x^{|H|}\phi(H,i/x)\right| \\
&= \mathrm{En}(H\setminus v) .
\end{aligned}$$

In particular, if we take H to be a fixed graph with cyclomatic number k, we can immediately deduce the following theorem:

Theorem 9 *For any positive integer k, there exists a constant b_k such that there are infinitely many graphs G with cyclomatic number k and the property that*

$$\mathrm{En}(G) \le 2\sqrt{|G|} + b_k \ .$$

Now we aim to apply the same idea to obtain graphs whose energy is close to $4n/\pi$. Let $P(\ell)$ be defined as in Section 2. Lemma 7 yields

$$\phi(P(\ell), x) = x\phi(P(\ell-1), x) - \phi(P(\ell-2), x) \ .$$

Define $\lambda(G, x) = (x/i)^{|G|} \cdot \phi(G, i/x)$. Then the recursion becomes

$$\lambda(P(\ell), x) = \lambda(P(\ell-1), x) + x^2\lambda(P(\ell-2), x) \ .$$

The solution to this linear recursion is given by

$$\lambda(P(\ell), x) = \beta_1(x)\alpha_1(x)^\ell + \beta_2(x)\alpha_2(x)^\ell \ ,$$

where $\alpha_1(x) = (1+\sqrt{1+4x^2})/2$, $\alpha_2(x) = (1-\sqrt{1+4x^2})/2$ and

$$\beta_1(x) = \frac{\lambda(P(1), x) - \alpha_2(x)\lambda(P(0), x)}{\alpha_1(x) - \alpha_2(x)} \ , \qquad \beta_2(x) = \frac{\alpha_1(x)\lambda(P(0), x) - \lambda(P(1), x)}{\alpha_1(x) - \alpha_2(x)} \ .$$

Note here also that $\alpha_1(x) - \alpha_2(x) = \sqrt{1+4x^2}$ is never 0. Hence the energy of $P(\ell)$ is given by

$$\begin{aligned}
\mathrm{En}(P(\ell)) &= \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2} \log\left|x^n\phi(P(\ell), i/x)\right| \\
&= \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2} \log\left|\lambda(P(\ell), x)\right| \\
&= \frac{2\ell}{\pi}\int_0^\infty \frac{dx}{x^2} \log\alpha_1(x)\, dx + \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left|\beta_1(x) + \beta_2(x)(\alpha_2(x)/\alpha_1(x))^\ell\right| \ .
\end{aligned}$$

The first integral is easily determined to be equal to 2. Moreover, for every fixed $x \ge 0$, the absolute value of $\alpha_2(x)/\alpha_1(x)$ is less than 1. So as we let ℓ tend to ∞, we obtain

$$\lim_{\ell\to\infty}\left(\mathrm{En}(P(\ell)) - \frac{4\ell}{\pi}\right) = \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log|\beta_1(x)| \ .$$

The integral converges, since $\beta_1(x)$ only grows polynomially and since $\lambda(P(\ell), x) = 1 + O(x^2)$, $\lambda(P(\ell), x) = 1 + O(x^2)$ and $\alpha_1(x) - \alpha_2(x) = \sqrt{1+4x^2} = 1 + O(x^2)$ imply $\beta_1(x) = 1 + O(x^2)$.

To justify that exchanging the integral and the limit is indeed always possible, we first show that $\beta_1(x)$ cannot have any positive real zeros: suppose that x_0 is the smallest such zero. Choose $x_1 < x_0$ large enough so that $\alpha_1(x_1) > |\alpha_2(x_0)|$. Then for sufficiently large ℓ, it follows that $|\lambda(P(\ell), x_1)| > |\lambda(P(\ell), x_0)|$. However, since $\lambda(P(\ell), x) = (x/i)^{|G|} \cdot \phi(G, i/x)$ has only purely imaginary zeros (the zeros of ϕ all being real), it can be factored into factors of the form $1 + cix$, from which it follows easily that $|\lambda(P(\ell), x)|$ is increasing, contradiction. So $|\beta_1(x)|$ is bounded below by a positive constant on any finite interval $[0, M]$, which implies that the integrand converges uniformly on such an interval. On the remaining interval, on the other hand, we can use dominated convergence, since $\beta_1(x) + \beta_2(x)(\alpha_1(x)/\alpha_2(x))^\ell$ is bounded by a polynomial in x, which means that the integrand is bounded by a constant multiple of the integrable function $x^{-2} \log x$.

So we can finally formulate a theorem analogous to Theorem 9:

Theorem 10 *For any positive integer k, there exists a constant a_k such that there are infinitely many graphs G with cyclomatic number k and the property that*

$$\mathrm{En}(G) \geq \frac{4n}{\pi} + a_k \ .$$

The construction also shows that Corollary 2 remains correct if "maximum" is replaced by "second-largest", "third-largest", etc. (and likewise for Theorem 3).

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