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# APPROXIMATIONS FOR VON NEUMANN AND RÉNYI ENTROPIES OF GRAPHS USING THE EULER-MACLAURIN FORMULA*

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**Abstract.** There have been many attempts of understanding graph structures by investigating graph entropies. In this article we investigate approximations for von Neumann and Rényi-$\alpha$ entropies of paths and rings, using the Euler-Maclaurin summation formula. For $\alpha$ an integer, the approximations become exact, and, in general, the obtained estimates have a remarkable degree of accuracy.

**Key words.** entropy, graphs, Laplacian matrix, Euler-Maclaurin formula

**AMS subject classifications.** 05C50, 81P45, 91A17

**1. Introduction.** The *Euler-Maclaurin (E-M) formula* is an important tool in numerical analysis and one of the most remarkable formulas in mathematics. It estimates a sum $\sum_{k=0}^{n} g(k)$ through the integral $\int_0^n g(t)\,\mathrm{d}t$ with an error term involving *Bernoulli numbers* [13]. One form of the E-M formula states

$$\sum_{k=0}^{n-1} g(k) = \int_0^n g(t)\,\mathrm{d}t - \frac{1}{2}(g(n)-g(0)) + \frac{1}{12}(g'(n)-g'(0)) - \frac{1}{2}\int_0^n B_2(\{t\})g''(t)\,\mathrm{d}t, \tag{1.1}$$

where $k$ is a nonnegative integer, $B_2(x) = x^2 - x + 1/6$ is the *second Bernoulli polynomial*, and $\{t\}$ denotes the fractional part of $t$. The condition imposed on the real function $g$ is that it should have a continuous second derivative for $t \in (0, n)$. If $g$ has a continuous second derivative for $t \in [0, n]$ and a continuous third derivative for $t \in (0, n)$, then the following form holds (see [8]):

$$\sum_{k=0}^{n-1} g(k) = \int_0^n g(t)\,\mathrm{d}t - \frac{1}{2}(g(n)-g(0)) + \frac{1}{12}(g'(n)-g'(0)) + \frac{1}{6}\int_0^n B_3(\{t\})g'''(t)\,\mathrm{d}t, \tag{1.2}$$

where $B_3(x) = x^3 - 3x^2/2 + x/2$ is the third Bernoulli polynomial.

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Under the weaker hypothesis that $g'(0)$ or $g'(n)$ do not exist, i.e., $g'(t)$ exists only for $t \in (0, n)$, instead of (1.1) the following holds:

$$\sum_{k=0}^{n-1} g(k) = \int_0^n g(t)\,\mathrm{d}t - \frac{1}{2}(g(n) - g(0)) + \int_0^n B_1(\{t\})g'(t)\,\mathrm{d}t, \tag{1.3}$$

where $B_1(x) = x - 1/2$ is the first Bernoulli polynomial.

In this paper we discuss the application of the E-M formula in graph entropy. The E-M formula is an important tool for numerical integration and numerical summation [14]. *Mathematica* also uses this famous formula [14, p. 917]. Interestingly, neither Euler nor Maclaurin presented this formula with remainder. The first one to do so was Poisson in 1830. Since then, it has been derived in different ways (see [1] and [8] for elementary derivations).

The notion of entropy is due to Rudolf Clausius (1850) and is connected with his famous theorem which generalizes the equally famous Carnot Theorem on the efficiency of thermal machines. The concept has gained many applications in several research areas such as statistical mechanics, information theory, etc. Recently, there have been many attempts of understanding graph structures by investigating graph entropies (see [3, 4, 12, 15] and references therein).

Let $G$ be an undirected graph with $n$ vertices and at least one edge, and let $L(G)$ be the *combinatorial Laplacian matrix* of $G$, that is, $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix whose $(i, i)$-th entry is the degree of the vertex $i$ and $A(G)$ is the *adjacency matrix* of $G$ [6]. Note that each row (and column) sum of $L(G)$ is 0, and so $L(G)$ is singular. Normalizing this matrix by its trace, we get

$$\rho(G) = \frac{1}{\operatorname{Tr} L(G)} L(G),$$

called the *density matrix of* $G$. By the *Gershgorin Theorem*, all eigenvalues of $\rho(G)$ are nonnegative [7]. Thus, $G$ can be seen as a quantum state since $\rho(G)$ is a Hermitian positive semidefinite matrix with unit trace. Therefore, it is natural to investigate the information content of the graph as a quantum state [10].

Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $\rho(G)$. Note that

$$\lambda_1 + \cdots + \lambda_n = 1.$$

The *von Neumann* entropy of $G$ is defined as

$$S(G) = -\sum_{i=1}^{n} \lambda_i \log_2 \lambda_i.$$

From now on, we will use the natural logarithm in the definitions of the entropy. (The two definitions, using $\log_2$ or $\log$, are equivalent up to a positive constant.) We make the convention that $0 \log 0 = 0$. We will use the following notations for a graph on $n$ vertices: $K_{1,n-1}$ denotes the *star graph*, $P_n$ denotes the *path*, $C_n$ denotes the *ring*, and $K_n$ denotes the *complete graph*.

It is well known that the Laplacian spectrum of the star graph is

$$\sigma(L(K_{1,n-1})) = \{0, n, 1, \ldots, 1\},$$

where the eigenvalue $1$ has multiplicity $n - 2$. Thus, we have

$$S(K_{1,n-1}) = \log(2n - 2) - \frac{n}{2n - 2} \log(n), \tag{1.4}$$

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and

$$\lim_{n\to\infty} \frac{S(K_{1,n-1})}{\log(n-1)} = \frac{1}{2}.$$

In [3, Conjecture 1.3], it has been conjectured that

CONJECTURE 1.1. *For all connected graphs $G$ on $n$ vertices,*

$$S(K_{1,n-1}) \leq S(G).$$

The conjecture was proved for almost all graphs with $n$ vertices [3, Theorem 2.3]. In the same article the following conjecture was also formulated:

CONJECTURE 1.2. *For any tree $T$ on $n$ vertices,*

$$S(T) \leq S(P_n).$$

Let $G$ be a graph with at least one edge. Consider the *density matrix* $\rho(G)$. For $\alpha \in (0,1)\cup(1,\infty)$ fixed, the *Rényi-$\alpha$ entropy* of $G$ [11] is defined as

$$H_\alpha(G) = \frac{1}{1-\alpha}\log\sum_{i=1}^{n}\lambda_i^\alpha$$

and is also denoted as $H_\alpha(\rho(G))$. For a fixed graph $G$, the Rényi-$\alpha$ entropy $H_\alpha(G)$ is a monotonically decreasing function of $\alpha$ [3],

$$H_\alpha(G) \leq H_{\alpha'}(G) \qquad \text{for } \alpha > \alpha'.$$

It was proved in [3, Proposition 3.1] that $H_\alpha(\lambda)$, for $\alpha > 1$ and $n \geq 1$, when viewed as a function of a probability distribution, $\lambda = (\lambda_1, \ldots, \lambda_n)$

1. is minimized by the distribution $\lambda_0 = (1, 0, \ldots, 0)$, and this is the only probability distribution (up to a permutation of the entries) that does so;
2. is maximized by the constant distribution $\lambda_c = (1/n, \ldots, 1/n)$.

We have

$$H_\alpha(K_{1,n-1}) = (1-\alpha)^{-1}\log((n^\alpha + n - 2)(2n-2)^{-\alpha}). \tag{1.5}$$

In [3, Conjecture 3.3], the following conjecture has been formulated.

CONJECTURE 1.3. *For $\alpha > 1$ and any connected graph $G$ on $n$ vertices,*

$$H_\alpha(K_{1,n-1}) \leq H_\alpha(G).$$

Note that, as

$$\lim_{\alpha\to 1^+} H_\alpha(G) = S(G),$$

the veracity of Conjecture 1.3 implies that Conjecture 1.1 has a positive answer.

This article is organized as follows: In Section 2 some useful background is presented. In Section 3, estimates of the Rényi-$\alpha$ entropy of paths and rings on $n$ vertices are obtained for $\alpha \in (1,\infty)$. The obtained approximations are shown to be exact in the case of $\alpha$ being an integer. In Section 4, approximations for the von Neumann entropy are given. The key tool for obtaining these estimates is the E-M formula. In Section 5, some final remarks are presented.

**2. Preliminary results.** Given a path $P_n$, up to a permutation similarity, $L(P_n)$ is the tridiagonal matrix

$$L(P_n) = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & & \\ 0 & -1 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 2 & -1 \\ 0 & & \cdots & -1 & 1 \end{bmatrix}. \tag{2.1}$$

The eigenvalues of $L(P_n)$ are well known in the literature and can be readily obtained [6].

LEMMA 2.1. *Let $P_n$ be a path on $n$ vertices. Then the eigenvalues of $L(P_n)$ are*

$$\beta_k = 2 + 2\cos(k\pi/n), \qquad k = 1, \dots, n.$$

The Laplacian matrix of the ring $C_n$ is the circulant matrix

$$L(C_n) = \begin{bmatrix} 2 & -1 & 0 & & -1 \\ -1 & 2 & -1 & & \\ 0 & -1 & \ddots & \ddots & \\ & & \ddots & 2 & -1 \\ -1 & 0 & & -1 & 2 \end{bmatrix}.$$

LEMMA 2.2 ([4]). *The eigenvalues of $L(C_n)$ are*

$$\beta_k = 2 - 2\cos(2\pi k/n), \qquad k = 1, 2, \dots, n.$$

PROPOSITION 2.3. *The Rényi-2 entropies of $P_n$ and $C_n$ are, respectively,*

$$H_2(P_n) = 2\log(2n-2) - \log(6n-8) \qquad \textit{and} \qquad H_2(C_n) = 2\log(2n) - \log(6n).$$

*Proof.* Observing that $\operatorname{Tr} P_n = 2n-2$, $\operatorname{Tr} C_n = 2n$, by easy computations, we get

$$\sum_{k=1}^{n}\left(2 + 2\cos\frac{k\pi}{n}\right)^2 = 6n-8, \qquad \text{and} \qquad \sum_{k=1}^{n}\left(2 - 2\cos\frac{2k\pi}{n}\right)^2 = 6n,$$

and the result follows. ∎

**3. On the Rényi-$\alpha$ entropy of paths and rings.**

**3.1. Estimates for paths.** The main results in this section are Theorems 3.5 and 3.6. To prove them, some auxiliary lemmas are needed. We start by presenting them. Throughout the article, the following form of the E-M formula is used:

LEMMA 3.1. *Let $n$ be a positive integer, and let $f$ be a real function of class $C^2$ in $[0,1]$. Then*

$$\sum_{k=1}^{n} f(k/n) = n\int_0^1 f(x)\,\mathrm{d}x + \frac{1}{2}(f(1)-f(0)) + \frac{1}{12n}(f'(1)-f'(0)) + R_n, \tag{3.1}$$

*with*

$$R_n = \frac{1}{6n^2}\int_0^1 B_3(\{nx\})f'''(x)\,\mathrm{d}x, \tag{3.2}$$

*$B_3(x) = x^3 - 3x^2/2 + x/2$ the third Bernoulli polynomial, and $\{x\}$ the fractional part of $x$.*

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*Proof.* By the E-M formula (1.2), we have

$$\begin{aligned}\sum_{k=1}^{n} f(k/n) &= f(n/n) - f(0/n) + \sum_{k=0}^{n-1} f(k/n)\\ &= f(n/n) - f(0/n) + \int_0^n f(t/n)\,\mathrm{d}t - \frac{1}{2}(f(n/n) - f(0/n))\\ &\quad + \frac{1}{12}\frac{\mathrm{d}f(t/n)}{\mathrm{d}t}\Big|_{t=0}^{t=n} + \frac{1}{6}\int_0^n B_3(\{t\})\frac{\mathrm{d}^3(t/n)}{\mathrm{d}t^3}\,\mathrm{d}t\\ &= \int_0^n f(t/n)\,\mathrm{d}t + \frac{1}{2}(f(n/n) - f(0/n))\\ &\quad + \frac{1}{12}\frac{\mathrm{d}f(t/n)}{\mathrm{d}t}\Big|_{t=0}^{t=n} + \frac{1}{6}\int_0^n B_3(\{t\})\frac{\mathrm{d}^3 f(t/n)}{\mathrm{d}t^3}\,\mathrm{d}t.\end{aligned}$$

Changing variables $x = t/n$, the result follows. ∎

LEMMA 3.2. *Let* $f : \mathbb{R} \to \mathbb{R}$

$$f(x) \coloneqq (2 + 2\cos(\pi x))^{\alpha}, \quad \alpha \in \mathbb{R}.$$

*Then for* $R_n$ *in* (3.2) *and* $\alpha > 1$

$$\lim_{n\to\infty} nR_n = 0.$$

*Proof.* Notice that

$$\begin{aligned}f''(x) &= -\frac{\alpha\pi^2}{2}(2 + 2\cos(\pi x))^{\alpha}(1 - \alpha + \alpha\cos(\pi x))\sec^2(\pi x/2),\\ f'''(x) &= \frac{\alpha\pi^3}{2}(2 + 2\cos(\pi x))^{\alpha}(-1 + 3\alpha - \alpha^2 + \alpha^2\cos(\pi x))\sec^2(\pi x/2)\tan(\pi x/2)\end{aligned}$$

and that $f'''(x_0) = 0$ for

$$x_0 = \frac{1}{\pi}\arccos((1 - 3\alpha + \alpha^2)/\alpha^2),$$

where $f'''(x)$ changes sign. By easy computations and having (1.2) in mind, we find for $\alpha > 1$,

$$\begin{aligned}\int_0^1 |f'''(x)|\,\mathrm{d}x &= f''(0) + f''(1) - 2f''(x_0)\\ &= \frac{\alpha\left(-4^{\alpha} + \left(4^{\alpha} + 4\left(4 + 2/\alpha^2 - 6/\alpha\right)^{\alpha}\right)\alpha\right)\pi^2}{2(-1+\alpha)} \eqqcolon d_{\alpha}.\end{aligned}$$

Having in mind that

$$|B_3(x)| \le \frac{1}{12\sqrt{3}},$$

we get

$$|R_n| \le \frac{d_{\alpha}}{72\sqrt{3}\,n^2},$$

and the result follows. ∎

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Throughout, we use the following formula as given in *Mathematica*:

$$\int_0^1 (2+2\cos(2\pi x))^\alpha \,\mathrm{d}x = \frac{4^\alpha \Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} =: c_\alpha, \tag{3.3}$$

where $\alpha > -1/2$ and $\Gamma$ is the well-known *Gamma function*.

LEMMA 3.3. *For $\alpha > 1$, we have*

$$\lim_{n\to\infty} n\left(\sum_{k=1}^n (2+2\cos(k\pi/n))^\alpha - \frac{4^\alpha\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)}n + \frac{4^\alpha}{2}\right) = 0.$$

*Proof.* For $f(x) := (2+2\cos(\pi x))^\alpha$, we have $f(1) = 0$, $f(0) = 4^\alpha$, $f'(1) = 0$, $f'(0) = 0$. This function is of class $C^2$ in the interval $[0,1]$. By Lemma 3.1, we get

$$\begin{aligned}\sum_{k=1}^n (2+2\cos\pi k/n)^\alpha &= n\int_0^1 f(x)\,\mathrm{d}x + \frac{1}{2}(f(1)-f(0)) + \frac{1}{12n}(f'(1)-f'(0)) + R_n\\ &= n\frac{4^\alpha\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} - \frac{4^\alpha}{2} + R_n,\end{aligned}$$

where $nR_n \to 0$ as $n\to\infty$, by Lemma 3.2. ∎

In Table 3.1 we compare, for $n = 40$, the sum $\sum_{k=0}^n \beta_k^\alpha$, where $\beta_1,\dots,\beta_n$ are the eigenvalues of $L(P_n)$, its approximation $c_\alpha n - 4^\alpha/2$, and $R_n$. The vanishing values of $R_n$ suggest that, for $\alpha$ a positive integer, $R_n = 0$.

TABLE 3.1
*Comparing $\sum_{k=0}^n \beta_k$, $c_\alpha n - 4^\alpha/2$, and $R_n$, for $n = 40$.*

| $\alpha$ | $\sum_{k=0}^n \beta_k^\alpha$ | $c_\alpha n - 4^\alpha/2$ | $R_n$ |
|---|---|---|---|
| $3/2$ | 131.812 | 131.812 | $4.03876\times 10^{-6}$ |
| 2 | 232 | 232 | 0 |
| $5/2$ | 418.599 | 418.599 | $-1.1875\times 10^{-8}$ |
| 3 | 768 | 768 | 0 |
| $7/2$ | 1426.05 | 1426.05 | $7.7307\times 10^{-11}$ |
| 4 | 2672 | 2672 | 0 |
| $9/2$ | 5041.97 | 5041.97 | $9.09495\times 10^{-13}$ |
| 5 | 9568 | 9568 | 0 |

It is interesting to consider the case when $\alpha$ is an integer. For $\alpha = m \in \mathbb{Z}^+$, we may write

$$\begin{aligned}\frac{4^\alpha\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} &= \frac{4^m\Gamma(1/2+m)}{\sqrt{\pi}\Gamma(1+m)} = \frac{4^m(m-1/2)(m-3/2)\cdots 1/2}{m!}\\ &= \frac{2^m(2m-1)!!}{m!},\end{aligned}$$

where $(2m-1)!! = (2m-1)(2m-3)\cdots 1$.

LEMMA 3.4. *For $m, n \in \mathbb{Z}^+$,*

$$\sum_{l=1}^n (2+2\cos(\pi l/n))^m = n2^m\frac{(2m-1)!!}{m!} - \frac{4^m}{2}.$$

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*Proof.* For $t \in \mathbb{R}$ and $p, k \in \mathbb{Z}^+$, by the binomial theorem, the following identity holds:

$$(2 + 2\cos(t))^m = 2^m \sum_{p=0}^{m} \cos^p(t) \binom{m}{p}, \quad m \in \mathbb{Z}^+.$$

Considering $(\mathrm{e}^{it} + \mathrm{e}^{-it})/2 = \cos(t)$, we easily find, again by the binomial theorem, that

$$\left(\frac{\mathrm{e}^{it} + \mathrm{e}^{-it}}{2}\right)^p = \frac{1}{2^p} \sum_{k=0}^{p} \binom{p}{k} \mathrm{e}^{2ikt - itp} = \frac{1}{2^p} \sum_{k=1}^{p} \binom{p}{k} \cos(2kt - tp)$$

because $\binom{p}{k} = \binom{p}{p-k}$. Hence,

$$\cos^p(t) = \frac{1}{2^p} \sum_{k=0}^{p} \cos((2k - p)t) \binom{p}{k}.$$

As the sum of the $n$ roots of unity is zero,

$$\sum_{k=1}^{n} \mathrm{e}^{2iks\pi/n} = 0, \qquad 0 \neq s \in \mathbb{Z},$$

for $r = 2s$, $0 \neq s \in \mathbb{Z}$, we have

$$\sum_{k=1}^{n} \cos(\pi r k/n) = 0.$$

For $r = 2s + 1$, $s \in \mathbb{Z}$, it can be easily seen that

$$\sum_{k=1}^{n} \cos(\pi r k/n) = -1.$$

Thus,

$$\sum_{l=1}^{n} (2 + 2\cos(\pi l/n))^m = n2^m \sum_{q=0}^{[m/2]} \frac{m!}{2^{2q}(m - 2q)!q!q!} - 2^m \sum_{q=0}^{q_{\max}} \binom{m}{2q + 1},$$

where $q_{\max} = m/2 - 1$ if $m$ is even and $q_{\max} = (m - 1)/2$ if $m$ is odd.

The following identity holds (see [2]):

$$\sum_{q=0}^{[m/2]} \frac{m!}{2^{2q}(m - 2q)!q!q!} = \frac{(2m - 1)!!}{m!}.$$

We easily conclude that

$$2^m \sum_{q=0}^{q_{\max}} \binom{m}{2q + 1} = \frac{4^m}{2},$$

and the result follows. ∎

THEOREM 3.5. *For $\alpha$ an integer and $c_\alpha$ in (3.3), the E-M approximation*

$$nc_\alpha - \frac{4^\alpha}{20}$$

*to the sum*

$$\sum_{l=1}^{n}(2+2\cos(\pi l/n))^{\alpha}$$

*is exact.*

*Proof.* This is a simple consequence of Lemma 3.4. □

We recall that

$$H_\alpha(P_n)=\frac{1}{1-\alpha}\left(\log\sum_{k=1}^{n}\beta_k^{\alpha}-\alpha\log(2n-2)\right), \tag{3.4}$$

where the $\beta_k$ are the eigenvalues of $L(P_n)$ in (2.1). We use the notation

$$\widetilde{H}_\alpha(P_n)=\frac{1}{1-\alpha}\left(\log\left(\frac{4^\alpha\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)}n-\frac{4^\alpha}{2}\right)-\alpha\log(2n-2)\right). \tag{3.5}$$

THEOREM 3.6. *For $\alpha>1$ and $\widetilde{H}_\alpha(P_n)$ in (3.5), we have*

$$\lim_{n\to\infty} n(H_\alpha(P_n)-\widetilde{H}_\alpha(P_n))=0.$$

*Further, it holds that*

$$\lim_{n\to\infty}\frac{H_\alpha(P_n)}{\log(n-1)}=1.$$

*Proof.* Let $\beta_1,\ldots,\beta_n$ be the eigenvalues of $L(P_n)$. We may write

$$H_\alpha(P_n)=\frac{1}{(1-\alpha)}\left(\log\sum_{i=1}^{n}\beta_i^{\alpha}-\alpha\log(2n-2)\right) \tag{3.6}$$

$$=\frac{1}{1-\alpha}\left(\log\left(\frac{4^\alpha\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)}n-\frac{4^\alpha}{2}+R_n\right)-\alpha\log(2n-2)\right) \tag{3.7}$$

so that for $c_\alpha$ in (3.3) we find

$$n(H_\alpha(P_n)-\widetilde{H}_\alpha(P_n))=\frac{1}{1-\alpha}\left(\log\left(c_\alpha n-\frac{4^\alpha}{2}+R_n\right)^n-\log\left(c_\alpha n-\frac{4^\alpha}{2}\right)^n\right)$$
$$=\frac{1}{1-\alpha}\left(\log\left(1+\frac{R_n}{c_\alpha n-4^\alpha/2}\right)^n\right).$$

We have

$$\lim_{n\to\infty}\log\left(1+\frac{R_n}{c_\alpha n-4^\alpha/2}\right)^n=\log\lim_{n\to\infty}\left(1+\frac{R_n}{n(c_\alpha-4^\alpha/(2n))}\right)^n=0$$

because $\lim_{n\to\infty}\frac{R_n}{c_\alpha-4^\alpha/(2n)}=0$. It follows that

$$\lim_{n\to\infty} n(H_\alpha(P_n)-\widetilde{H}_\alpha(P_n))=0.$$

We may also write

$$H_\alpha(P_n)=\log(n-1)+\frac{\log(c_\alpha+(c_\alpha-4^\alpha/2+R_n)/(n-1))-\alpha\log 2}{1-\alpha}$$

so that

$$\frac{H_\alpha(P_n)}{\log(n-1)}=1+\frac{\log\left(c_\alpha+(c_\alpha-4^\alpha/2+R_n)/(n-1)\right)-\alpha\log 2}{(1-\alpha)\log(n-1)}.$$

Then, the last statement follows. □

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TABLE 3.2
*Comparing $H_{3/2}(P_n)$, $\widetilde{H}_{3/2}(P_n)$, $H_{3/2}(K_{1,n-1})$, and $nR_n$.*

| $n$ | $H_{3/2}(P_n)$ | $\widetilde{H}_{3/2}(P_n)$ | $H_{3/2}(K_{1,n-1})$ | $nR_n$ |
|---|---|---|---|---|
| 5 | 1.111 714 14 | 1.112 040 36 | 0.934 611 644 | 0.010 583 9 |
| 10 | 1.871 835 31 | 1.871 852 66 | 1.312 307 03 | 0.002 599 12 |
| 20 | 2.597 927 55 | 2.597 928 56 | 1.558 842 76 | 0.000 646 914 |
| 40 | 3.307 369 78 | 3.307 369 84 | 1.723 602 20 | 0.000 161 550 |
| 80 | 4.008 615 81 | 4.008 615 82 | 1.834 772 78 | 0.000 040 376 5 |
| 160 | 4.705 799 76 | 4.705 799 76 | 1.910 290 25 | 0.000 010 093 5 |

**3.1.1. Numerical experiments.** In Table 3.2 we compare the Rényi-$3/2$ entropy of the path $P_n$ with the approximate result in Theorem 3.6, denoted by $\widetilde{H}_{3/2}(P_n)$, and with the Rényi-$3/2$ entropy of $K_{1,n-1}$ using equations (3.4), (3.5), and (1.5). The values of $nR_n$ are also presented, suggesting that $nR_n$ behaves like $1/n^2$ so that $R_n$ behaves like $1/n^3$.

Notice that (3.5), which has been derived having (1.1) in mind, remains valid also if $\alpha < 1$. In this case, we use (1.3), the only difference is the so obtained $R_n$ because in the actual application of the formula it turns out that $g'(n) = g'(0) = 0$.

In Table 3.3 we compare the Rényi-$1/2$ entropy of the path $P_n$ with $\widetilde{H}_{1/2}(P_n)$ and with the Rényi-$1/2$ entropy of $K_{1,n-1}$ using equations (3.4), (3.5), and (1.5). The values of $nR_n$ are also presented, suggesting that $nR_n$ remains almost constant so that $R_n$ behaves like $1/n$.

TABLE 3.3
*Comparing $H_{1/2}(P_n)$, $\widetilde{H}_{1/2}(P_n)$, $H_{1/2}(K_{1,n-1})$, and $nR_n$.*

| $n$ | $H_{1/2}(P_n)$ | $\widetilde{H}_{1/2}(P_n)$ | $H_{1/2}(K_{1,n-1})$ | $nR_n$ |
|---|---|---|---|---|
| 5 | 1.261 154 63 | 1.280 797 66 | 1.231 700 12 | −0.262 231 |
| 10 | 2.029 866 28 | 2.034 335 96 | 1.934 708 30 | −0.261 907 |
| 20 | 2.755 813 29 | 2.756 883 80 | 2.586 966 12 | −0.261 826 |
| 40 | 3.464 256 28 | 3.464 518 47 | 3.226 368 81 | −0.261 806 |
| 80 | 4.164 790 32 | 4.164 855 21 | 3.867 939 69 | −0.261 801 |
| 160 | 4.861 567 40 | 4.861 583 55 | 4.517 167 54 | −0.261 800 |

TABLE 3.4
*Comparing $H_{1/4}(P_n)$, $\widetilde{H}_{1/4}(P_n)$, $H_{1/4}(K_{1,n-1})$, and $\sqrt{n}R_n$.*

| $n$ | $H_{1/4}(P_n)$ | $\widetilde{H}_{1/4}(P_n)$ | $H_{1/4}(K_{1,n-1})$ | $\sqrt{n}R_n$ |
|---|---|---|---|---|
| 5 | 1.318 667 98 | 1.366 411 22 | 1.310 910 50 | −0.368 592 936 |
| 10 | 2.101 769 31 | 2.117 273 19 | 2.076 760 80 | −0.368 499 782 |
| 20 | 2.833 087 94 | 2.838 363 06 | 2.789 408 62 | −0.368 476 500 |
| 40 | 3.543 421 84 | 3.545 253 41 | 3.483 322 38 | −0.368 470 680 |
| 80 | 4.244 573 58 | 4.245 215 50 | 4.171 580 73 | −0.368 469 225 |
| 160 | 4.941 530 05 | 4.941 756 03 | 4.859 123 26 | −0.368 468 861 |

In Table 3.4 we compare the Rényi-$1/4$ entropy of the path $P_n$ with $\widetilde{H}_{1/4}(P_n)$ and with the Rényi-$1/4$ entropy of $K_{1,n-1}$ using (3.4), (3.5), and (1.5). The values of $\sqrt{n}R_n$ are also presented, suggesting that $\sqrt{n}R_n$ remains almost constant so that $R_n$ behaves like $1/\sqrt{n}$.

**3.2. Estimates for rings.** Next we state results for rings analogous to those previously presented for paths. We omit the proofs since they are similar.

LEMMA 3.7. *Let $\alpha > 1$ and $f : \mathbb{R} \to \mathbb{R}$ be defined by $f(x) := (2 - 2\cos(2\pi x))^{\alpha}$. Then*

$$\lim_{n\to\infty} n \left( \sum_{k=1}^{n} f(\frac{k}{n}) - n\frac{4^{\alpha}\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} \right) = 0.$$

*Proof.* The proof is similar to the one of Lemma 3.3. □

Notice that

$$H_{\alpha}(C_n) = \frac{1}{1-\alpha} \left( \log \left( n\frac{4^{\alpha}\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} + R_n \right) - \alpha \log(2n) \right). \tag{3.8}$$

We use the notation

$$\widetilde{H}_{\alpha}(C_n) = \frac{1}{1-\alpha} \left( \log \left( n\frac{4^{\alpha}\Gamma(1/2+\alpha)}{\sqrt{\pi}\Gamma(1+\alpha)} \right) - \alpha \log(2n) \right). \tag{3.9}$$

THEOREM 3.8. *For $\alpha > 1$,*

$$\lim_{n\to\infty} n(H_{\alpha}(C_n) - \widetilde{H}_{\alpha}(C_n)) = 0,$$

*with $H_{\alpha}(C_n)$ and $\widetilde{H}_{\alpha}(C_n)$ in (3.8) and (3.9), respectively. Moreover, the approximation for integer values of $\alpha$ becomes exact, and*

$$\lim_{n\to\infty} \frac{H_{\alpha}\left(C_n\right)}{\log(n-1)} = 1.$$

*Proof.* The proof is similar to those of Theorems 3.5 and 3.6. □

In Table 3.5 we compare, $H_{3/2}(C_n)$, $\widetilde{H}_{3/2}(C_n)$, and $H_{3/2}(K_{1,n-1})$ using (3.8), (3.9), and (1.5). The last column suggests that $nR_n$ behaves like $1/n^2$ so that $R_n$ behaves like $1/n^3$.

TABLE 3.5
*Comparing $H_{3/2}(C_n)$, $\widetilde{H}_{3/2}(C_n)$, $H_{3/2}(K_{1,n-1})$, and $nR_n$.*

| $n$ | $H_{3/2}(C_n)$ | $\widetilde{H}_{3/2}(C_n)$ | $H_{3/2}(K_{1,n-1})$ | $nR_n$ |
|---|---|---|---|---|
| 5 | 1.239 797 86 | 1.244 092 00 | 0.934 611 644 | 0.182 445 |
| 10 | 1.936 989 82 | 1.937 239 18 | 1.312 307 03 | 0.042 335 5 |
| 20 | 2.630 371 05 | 2.630 386 36 | 1.558 842 76 | 0.010 396 5 |
| 40 | 3.323 532 59 | 3.323 533 54 | 1.723 602 20 | 0.002 587 66 |
| 80 | 4.016 680 66 | 4.016 680 72 | 1.834 772 78 | 0.000 646 201 |
| 160 | 4.709 827 90 | 4.709 827 90 | 1.910 290 25 | 0.000 161 506 |

**4. Estimating the von Neumann entropy of paths and rings.** In this section we apply the E-M formula to the evaluation of the von Neumann entropy of the path $P_n$ for arbitrary $n$.

Let $f : \mathbb{R} \to \mathbb{R}$,

$$f(x) := (2 + 2\cos(\pi x)) \log(2 + 2\cos(\pi x)).$$

Then (3.1) and (3.2) hold. Since $f(x)$ is not of class $C^2$ in $[0, 1]$, the upper bound for $R_n$ in (1.2) is not useful. However, it holds that

$$\lim_{n\to\infty} R_n = 0.$$

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Indeed, we clearly have

$$|R_n| \le \frac{1}{12n}\int_0^1 |f''(x)|\,\mathrm{d}x = \frac{2.41988}{n}$$

since, numerically, we find

$$\int_0^1 |f''(x)|\,\mathrm{d}x = 29.0386.$$

We estimate $R_n$. For this purpose, we consider the integral in (3.2)

$$\frac{1}{n}\int_0^1 B_2(\{nx\})f''(tx)\,\mathrm{d}x = \int_0^n B_2(\{t\})\frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2}\,\mathrm{d}t.$$

As $f(x)$ is not of class $C^2$ in $[0,1]$, we consider the form (1.1) of the E-M formula. In order to deal with a divergence which arises in the integral, we split the integral over $t$ into two parts:

$$\int_0^n B_2(\{t\})\frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2}\,\mathrm{d}t = \int_0^{n-1} B_2(\{t\})\frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2}\,\mathrm{d}t + \int_{n-1}^n B_2(\{t\})\frac{d^2 f(t/n)}{\mathrm{d}t^2}\,\mathrm{d}t.$$

By the version (1.3) of the E-M formula, the sum $\sum_{k=0}^{n-1} i(k)$ can be estimated by the integral $\int_0^n i(t)\,\mathrm{d}t$. To evaluate this integral, we consider

$$\int_0^{n-1} B_2(\{t\})\frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2}\,\mathrm{d}t.$$

The fourth derivative of $f(t/n)$ is given by

$$\frac{\mathrm{d}^4 f}{\mathrm{d}t^4} = \frac{\pi^4}{n^4}\left(-2+2\cos(\frac{\pi t}{n})\left(4+\log 2+\log\left(1+\cos(\frac{\pi t}{n})\right)\right) - \sec^2(\frac{\pi t}{2n})\right) =: g(t).$$

Thus,

$$\begin{aligned} i(k) &:= \int_k^{k+1} B_2(\{t\})\frac{d^2 f(t/n)}{\mathrm{d}t^2}\mathrm{d}t = \frac{1}{360}g(k) + \ldots \\ &= \frac{\pi^4}{360 n^4}\big(-2+2\cos(\pi k/n)\,(4+\log 2+\log\left(1+\cos(\pi k/n)\right)) \\ &\qquad - \sec^2(\pi k/(2n))\big) + O(1/n), \end{aligned}$$

where $O(1/n)$ approaches 0 as $n \to \infty$.

By changing variables $x = k/n$ in the integral we find that

$$\begin{aligned} &\int_0^{n-1} i(k)\,\mathrm{d}k = n\int_0^{(n-1)/n} i(nx)\,\mathrm{d}x \\ &= \frac{1}{360}\frac{1}{n^3}\int_0^{1-1/n} \pi^3\left(-2+2\cos(\pi x)(4+\log 2+\log(1+\cos(\pi x))) - \sec^2(\pi x/2)\right)\mathrm{d}x \\ &= -\frac{4\pi^2}{360 n^2}, \end{aligned}$$

if $n$ is sufficiently large.

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Next we evaluate

$$\int_{n-1}^{n} B_2(\{t\}) \frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2} \mathrm{d}t$$

using

$$\frac{\mathrm{d}^2 f}{\mathrm{d}k^2} = 6\pi^2 n^{-2} + 2\pi^2 n^{-2} \log\left(\left(\pi - \frac{k\pi}{n}\right)^2\right) + n^{-2} O(1/n),$$

which is valid for $n$ large and $k$ close to $n$. Hence, for $n$ large

$$\int_{n-1}^{n} B_2(\{t\}) \frac{\mathrm{d}^2 f(t/n)}{\mathrm{d}t^2}\, \mathrm{d}t = -\frac{\pi^2}{9n^2} + n^{-2} O(1/n)$$

and

$$R_n = \frac{2\pi^2}{360n^2} + \frac{\pi^2}{18n^2} + O(1/n^3) = \frac{11\pi^2}{180n^2} + O(1/n^3).$$

Thus $\lim_{n\to\infty} nR_n = 0$, and so

$$\lim_{n\to\infty} n \left(\sum_{k=1}^{n} f\left(\frac{k}{n}\right) - 2n + 2\log 4\right) = 0.$$

The entropy of the path $P_n$ is given by

$$S(P_n) = \log(2n-2) - \frac{1}{2n-2} \sum_{i=1}^{n} \beta_i \log \beta_i, \tag{4.1}$$

where $\beta_1, \ldots, \beta_n$ are the eigenvalues of $L(P_n)$ in (2.1). By the formula of Euler-Maclaurin, we may write as in the Lemma 3.1

$$S(P_n) = \log(2n-2) - \frac{1}{2n-2} \left(2n - 4\log 2 + R_n\right). \tag{4.2}$$

We have

$$S(P_n) - \widetilde{S}(P_n) = -\frac{1}{2n-2} R_n,$$

where

$$\widetilde{S}(P_n) = \log(2n-2) - \frac{1}{2n-2} \left(2n - 4\log 2\right).$$

Now,

$$\lim_{n\to\infty} n \left(S(P_n) - \widetilde{S}(P_n)\right) = 0,$$

and further, since

$$\frac{S(P_n)}{\log(n-1)} = 1 + \frac{1}{\log(n-1)} \left(\log(2) - \frac{1}{2n-2} \left(2n - 4\log 2 + R_n\right)\right),$$

TABLE 4.1
*Comparing $S(P_n)$, $\widetilde{S}(P_n)$, $S(K_{1,n-1})$, and $nR_n$.*

| $n$ | $S(P_n)$ | $\widetilde{S}(P_n)$ | $S(K_{1,n-1})$ | $nR_n$ |
|---|---|---|---|---|
| 5 | 1.172 983 81 | 1.176 015 13 | 1.073 542 85 | 0.121 253 |
| 10 | 1.932 958 73 | 1.933 293 35 | 1.611 157 82 | 0.060 232 8 |
| 20 | 2.657 877 88 | 2.657 917 44 | 2.060 884 96 | 0.030 067 6 |
| 40 | 3.366 608 99 | 3.366 613 81 | 2.464 975 77 | 0.015 027 7 |
| 80 | 4.067 484 24 | 4.067 484 84 | 2.843 847 37 | 0.007 513 11 |
| 160 | 4.764 480 83 | 4.764 480 91 | 3.208 504 81 | 0.003 756 46 |

it follows that

$$\lim_{n\to\infty} \frac{S\left(P_n\right)}{\log(n-1)} = 1.$$

In Table 4.1 we compare the von Neumann entropy of the path $P_n$ with the approximate result denoted by $\widetilde{S}(P_n)$ and with the von Neumann entropy of $K_{1,n-1}$ using equations (4.1), (4.2), and (1.4). The values of $nR_n$ are also presented, indicating that $nR_n$ behaves like $1/n$ so that $R_n$ behaves like $1/n^2$. We notice that $\widetilde{S}(P_n)$ approaches $S(P_n)$ from above.

We next obtain similar results for the ring $C_n$ with $n$ vertices. Consider the function $f:\mathbb{R}\to\mathbb{R},\ f(x) := (2-2\cos(2\pi x))\log(2-2\cos(2\pi x))$, observe that $f(1)-f(0)=0$, $f'(1)-f'(0)=0$, and that

$$\int_0^1 f(x)\log f(x)\,\mathrm{d}x = 2,$$

as given by *Mathematica*. By Lemma 3.1, we obtain

$$S(C_n) = \log(2n) - \frac{1}{2n}(2n+R_n). \tag{4.3}$$

As $\lim_{n\to\infty} nR_n = 0$, we have

$$\lim_{n\to\infty}(S(C_n) - \widetilde{S}(C_n)) = 0,$$

where

$$\widetilde{S}(C_n) = \log(2n) - 1. \tag{4.4}$$

Moreover,

$$\lim_{n\to\infty} \frac{S(C_n)}{\log(n-1)} = 1.$$

In Table 4.2 we compare the von Neumann entropy of the ring $C_n$ with the approximation $\widetilde{S}(C_n)$ and with the von Neumann entropy of $K_{1,n-1}$ using (4.3), (4.4), and (1.4). The last column suggests that $nR_n$ behaves like $1/n$ so that $R_n$ behaves like $1/n^2$.

**5. Final remarks.** In this note we have illustrated applications of the Euler-Maclaurin formula to the estimation of graph entropies of paths and rings. More generally, E-M formulas are available and potentially can be used in the same way as it was done for entropies of other graphs. From the previous Theorems 3.6 and 3.8 we conclude that, asymptotically, $H_\alpha(P_n)$ and $H_\alpha(C_n)$ behave as $\log(n-1)$.

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TABLE 4.2
*Comparing $S(C_n)$, $\widetilde{S}(C_n)$, $S(K_{1,n-1})$, and $nR_n$.*

| $n$ | $S(C_n)$ | $\widetilde{S}(C_n)$ | $S(K_{1,n-1})$ | $nR_n$ |
|---|---|---|---|---|
| 5 | 1.282 661 67 | 1.302 585 09 | 1.073 542 85 | 0.996 171 |
| 10 | 1.993 307 22 | 1.995 732 27 | 1.611 157 82 | 0.485 011 |
| 20 | 2.688 578 29 | 2.688 879 45 | 2.060 884 96 | 0.240 931 |
| 40 | 3.381 989 05 | 3.382 026 63 | 2.464 975 77 | 0.120 271 |
| 80 | 4.075 169 12 | 4.075 173 82 | 2.843 847 37 | 0.060 110 9 |
| 160 | 4.768 320 41 | 4.768 321 00 | 3.208 504 81 | 0.030 052 4 |

In Figure 5.1 we present $H_\alpha(P_n) - \widetilde{H}_\alpha(P_n)$ on the left-hand side and $R_n$ on the right-hand side for $2 \le n \le 160$ and for $\alpha = 1/2, 3/2, 5/2$ and $7/2$. It may be seen that $R_n$ and $H_\alpha(P_n) - \widetilde{H}_\alpha(P_n)$ decrease extremely fast in absolute value as $n$ increases. Indeed, these quantities are practically equal to 0 for $n > 30$.

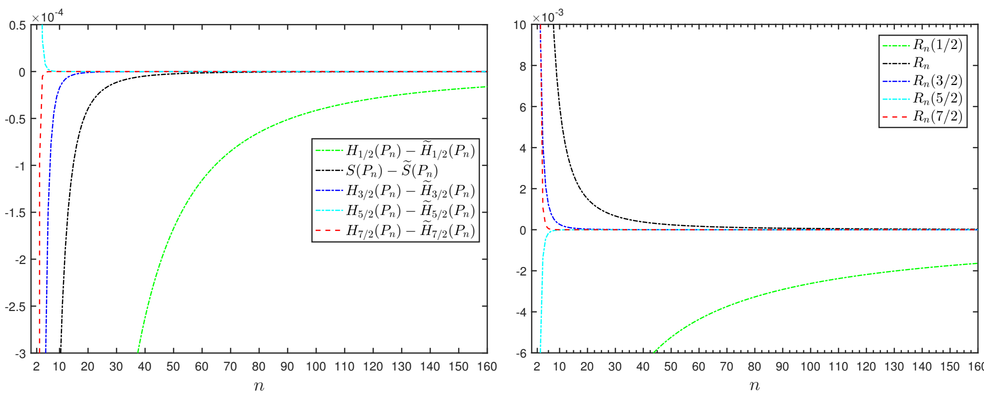


FIG. 5.1. *The behavior of $H_\alpha(P_n) - \widetilde{H}_\alpha(P_n)$ on the left-hand side and of the corresponding $R_n$ on the right-hand side as n increases. The curve labeled $R_n$ in the figure refers to the error in the sum $\sum_{k=1}^{n} \beta_k \log \beta_k$, where $\beta_k$ are the eigenvalues of* (2.1).

In Figure 5.3, we present the von Neumann entropy $\widetilde{S}(P_n)$ for the path $P_n$ and the Rényi-$\alpha$ entropies $\widetilde{H}_\alpha(P_n)$ for $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{2}, 2$. We can see from this figure that

$$\widetilde{H}_{1/4}(P_n) > \widetilde{H}_{1/2}(P_n) > \widetilde{S}(P_n) > \widetilde{H}_{3/2}(P_n) > \widetilde{H}_2(P_n)$$

as expected. These entropies increase with $n$ for $n \ge 2$.

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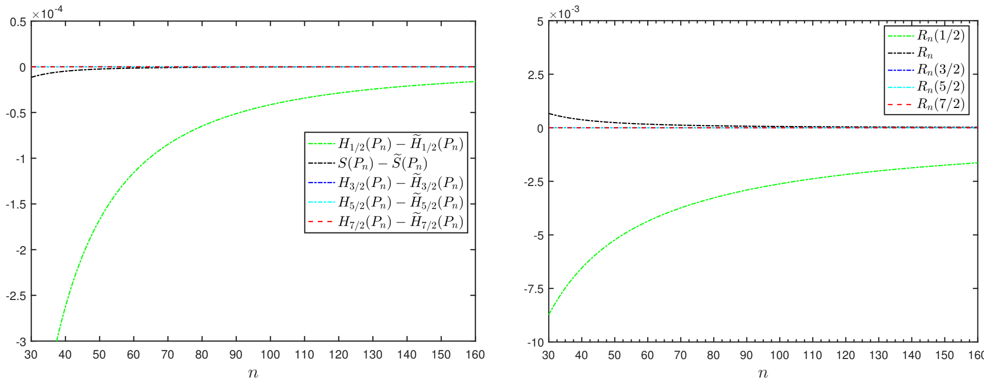


FIG. 5.2. *Enlarged detail of Figure 5.1.*

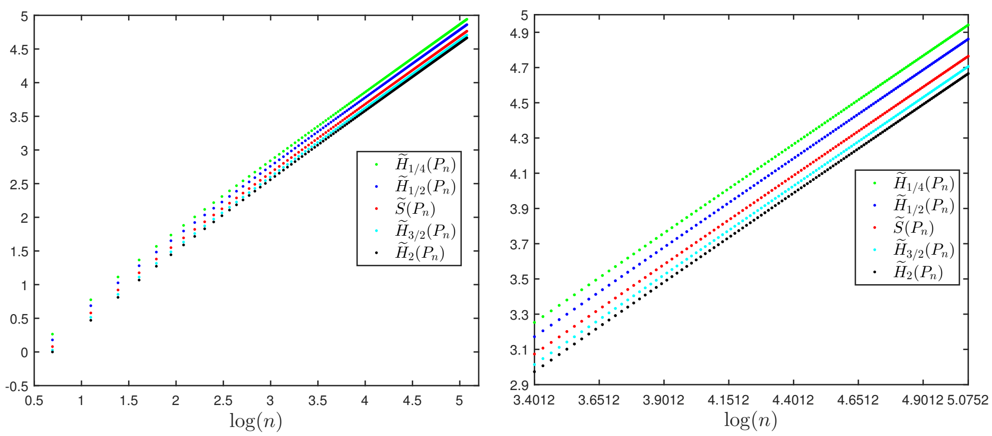


FIG. 5.3. *The Rényi-$\alpha$ entropies of the path $P_n$ for $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{2}$,2 and the entropy of the path $P_n$.*

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