THE TRACE METHOD FOR COTANGENT SUMS

WIKTOR EJSMONT AND FRANZ LEHNER

Abstract. This paper presents a combinatorial study of sums of integer powers of the cotangent which is a popular theme in classical calculus. Our main tool the realization of cotangent values as eigenvalues of a simple self-adjoint matrix with integer matrix. We use the trace method to draw conclusions about integer values of the sums and and provide explicit evaluations; it is remarkable that throughout the calculations the combinatorics are governed by the higher tangent and arctangent numbers exclusively. Finally we indicate a new approximation of the values of the Riemann zeta function at even integer arguments.

Contents

1. Introduction

It is a well known fact that the trace of a matrix equals the sum of its eigenvalues

$$\mathrm{Tr}\,A=\sum\lambda_i,$$

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counting algebraic multiplicities. This relation is respected by functional calculus and the identity

$$\operatorname{Tr} f(A) = \sum f(\lambda_i)$$

holds for arbitrary holomorphic (and other functions in the case of self-adjoint matrices), in particular, powers and polynomials. The *trace method* consists in the evaluation of this identity for particular matrices in order to obtain nontrivial combinatorial relations.
In the present paper we apply this method to cotangent sums of the form

$$\mathrm{S}(m,n,\alpha) = \sum_{k=0}^{n-1} \cot^m \frac{\alpha + k\pi}{n} \tag{1.1}$$

for $\alpha \neq k\pi$, $n, m \in \mathbb{N}$, $n \geqslant 2$, and the limit case

$$S_0(m,n) = \sum_{k=1}^{n-1} \cot^m \frac{k\pi}{n}. \tag{1.2}$$

Sums of this kind are a recurrent theme in the mathematical literature. They arise in number theory in connection with Dedekind sums and topology [50, 30], and more recently were used to evaluate the Riemann zeta function, see [49, Problem 141ff] for the apparently first occurrence of this connection and later rediscoveries [33, 47, 38, 6, 3, 21]; Berndt and Yeap [8] attribute the first occurence of cotangent sums to [45, p. 155]. The recent literature on this topic is abundant, in particular the question for which values of the parameters the sums (1.1) yield integer values is intriguing. For example, Byrne and Smith [11] proved that the sums are integer valued polynomials in n at the offset $\alpha = \pi/4$, found the leading terms and established recurrence relations. For the case $m = 2$ finite Fourier analysis is applicable [4]. We were led to study such sums in connection with certain limit theorems arising in free probability, see our papers [24, 23], where the matrices considered below arise in a natural way and we apply the trace method and expansions of generating functions to evaluate such expressions into closed form.
We will see below that in many cases the integrity of the values of (1.1) is a simple consequence of the trace formula; moreover we provide an explicit formula and as a corollary, the sums in terms of arctangent, tangent and secant numbers

$$S(2m+1,n,\pi/4) = \sum_{k=1}^{n} (-1)^k \cot^{2m+1} \frac{(2k-1)\pi}{4n} = \frac{1}{2(2m)!} \sum_{k=0}^{m} (2n)^{2k+1} A_{2m+1}^{(2k+1)}\, S_{2k},$$

$$S(2m,n,\pi/4) = \sum_{k=1}^{n} \cot^{2m} \frac{(2k-1)\pi}{4n} = (-1)^m n + \frac{1}{2(2m-1)!} \sum_{k=1}^{m} (2n)^{2k} A_{2m}^{(2k)}\, T_{2k-1},$$

see Corollary 6.4. Moreover we obtain an explicit formula for the sum (1.2)

$$\sum_{k=1}^{n-1} \cot^{2m} \frac{k\pi}{n} = (-1)^m (n-1) - \frac{1}{(2m-1)!} \sum_{k=1}^{m} (-1)^k A_{2m}^{(2k)} \frac{4^k B_{2k}}{2k} (n^{2k} - 1).$$

which was previously evaluated by Berndt and Yeap in terms of Bernoulli numbers [8] (cf. also [48, 27, 21, 2, 22, 29]), see Corollary 6.5. Chu and Marini [15] wrote a systematic study of generating functions and we complement this in Section 4 by providing a generating function for arbitrary α. The most general formula for the sum (1.1) so far was given in by Cvijović and Klinowski [20], who realized the cotangent values $\cot \frac{\alpha+k\pi}{n}$ as roots of a polynomial and expressed the sums via Cramer's rule applied to the Newton relations between elementary and power sum symmetric functions. In the present paper we go one step further and show that the polynomial found in [20] is in fact the characteristic polynomial of a simple matrix. Thus the trace method is applicable and we can draw certain conclusions about the sum (1.1). For example, if $\cot \alpha$ is an integer, e.g., $\alpha = \frac{\pi}{4}$, it follows trivially that (1.1) evaluates to an integer,

as was observed by different means in [11]. For an evaluation of cosecant sums via the trace method see [44].
It is perhaps interesting to note that the papers [12, 13] evaluate certain trigonometric sums using matrices with trigonometric entries and integer eigenvalues, while in the present paper we exploit integer matrices with trigonometric eigenvalues.

2. Preliminaries on Linear Algebra and the Tangent function

The main role in this paper is played by a certain matrix and its intricate relations to the tangent and cotangent functions.

2.1. **A matrix.** For scalars $a, b, c \in \mathbb{C}$ we denote by $\left[\begin{smallmatrix} a & b \\ c & a \end{smallmatrix}\right]_n \in M_n(\mathbb{C})$ the matrix whose diagonal elements are equal to a, whose upper-triangular entries are equal to b and whose lower-triangular elements are equal to c, respectively. For simplicity of notation, we use the same letter J_n and B_n for the following matrices

$$J_n := \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \ddots & 1 \\ \vdots & & \ddots & \ddots & \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix} \quad \text{and} \quad B_n := i \begin{bmatrix} 0 & 1 & 1 & \dots & 1 \\ -1 & 0 & 1 & \dots & 1 \\ -1 & -1 & 0 & \ddots & 1 \\ \vdots & & \ddots & \ddots & \\ -1 & -1 & -1 & \dots & 0 \end{bmatrix}.$$

The first observation reveals that the entries of the sum (1.1) can be realized as eigenvalues of the following matrix and consequently the sum is the trace of the m-th power of this matrix.

Lemma 2.1. *If $a = \cot\alpha$, then the characteristic polynomial of the matrix*

$$C_n = aJ_n + B_n = \begin{bmatrix} a & a+i & \dots & a+i \\ a-i & a & \dots & a+i \\ \dots & \dots & \dots & \dots \\ a-i & a-i & \dots & a \end{bmatrix} \in M_n(\mathbb{C})$$

is

$$\chi_n(\alpha;\lambda) = \frac{(\cot\alpha + i)(\lambda - i)^n - (\cot\alpha - i)(\lambda + i)^n}{2i} = \operatorname{Im}(\cot\alpha + i)(\lambda - i)^n \tag{2.1}$$

(assuming λ real) and the eigenvalues are given by

$$\lambda_k = \cot\frac{\alpha + k\pi}{n}, \ \textit{for } 0 \leqslant k \leqslant n-1.$$

Proof. The spectrum of the matrix C_n can be computed from its characteristic polynomial $\chi_n(\alpha;\lambda) = \det(\lambda I - C_n)$ using the following recurrence relation. Let $w = a + i$, then we have

$$\chi_n(\alpha;\lambda) = \begin{vmatrix} \lambda - a & -w & -w & -w & \dots & -w \\ -\overline{w} & \lambda - a & -w & -w & \dots & -w \\ -\overline{w} & -\overline{w} & \lambda - a & -w & \dots & -w \\ -\overline{w} & -\overline{w} & -\overline{w} & \lambda - a & \dots & -w \\ \dots & \dots & \dots & \dots & \dots & \dots \\ -\overline{w} & -\overline{w} & -\overline{w} & -\overline{w} & \dots & \lambda - a \end{vmatrix}$$

we subtract the second row from the first row

$$= \begin{vmatrix} \lambda - a + \overline{w} & -\lambda - w + a & 0 & 0 & \dots & 0 \\ -\overline{w} & \lambda - a & -w & -w & \dots & -w \\ -\overline{w} & -\overline{w} & \lambda - a & -w & \dots & -w \\ -\overline{w} & -\overline{w} & -\overline{w} & \lambda - a & \dots & -w \\ \dots & \dots & \dots & \dots & \dots & \dots \\ -\overline{w} & -\overline{w} & -\overline{w} & -\overline{w} & \dots & \lambda - a \end{vmatrix}$$

and the second column from the first column

$$= \begin{vmatrix} 2\lambda - 2a + w + \overline{w} & -\lambda - w + a & 0 & 0 & \dots & 0 \\ -\lambda - \overline{w} + a & \lambda - a & -w & -w & \dots & -w \\ 0 & -\overline{w} & \lambda - a & -w & \dots & -w \\ 0 & -\overline{w} & -\overline{w} & \lambda - a & \dots & -w \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & -\overline{w} & -\overline{w} & -\overline{w} & \dots & \lambda - a \end{vmatrix}$$
$$= (2\lambda - 2a + w + \overline{w})\chi_{n-1}(\alpha;\lambda) - (\lambda - a + w)(\lambda - a + \overline{w})\chi_{n-2}(\alpha;\lambda)$$

and the solution of this recurrence equation (with initial values $\chi_0(\alpha;\lambda) = 1$ and $\chi_1(\alpha;\lambda) = \lambda$) is

$$\begin{aligned} \chi_n(\alpha;\lambda) &= \frac{w(\lambda - a + \overline{w})^n - \overline{w}(\lambda - a + w)^n}{w - \overline{w}} \\ &= \frac{(a+i)(\lambda - i)^n - (a-i)(\lambda + i)^n}{2i} = \operatorname{Im}(a+i)(\lambda - i)^n. \end{aligned}$$

Thus we have to solve the equation

$$\operatorname{Im}(a+i)(\lambda - i)^n = 0. \tag{2.2}$$

To compute the zeros, write $a+i = r_0 e^{i\alpha}$, i.e., $a = \cot\alpha$ and assume $\lambda - i = re^{-i\theta}$. Then equation (2.2) becomes $\operatorname{Im} r_0 e^{i\alpha} r^n e^{-in\theta} = 0$ and is equivalent to the equation $\sin(\alpha - n\theta) = 0$, that is, $\alpha - n\theta = -k\pi$ for some $k \in \mathbb{Z}$. Thus the solutions of (2.2) can be written as $\lambda_k = i + r_k e^{-i\theta_k}$ with $\theta_k = \frac{\alpha + k\pi}{n}$. Now our matrix is selfadjoint, all roots of the characteristic polynomial (2.2) are real and hence $-1 = \operatorname{Im}(\lambda_k - i) = -r_k \sin\theta_k$; we conclude that $r_k = \frac{1}{\sin\theta_k}$ and $\lambda_k = \operatorname{Re}(\lambda_k - i) = r_k\cos\theta_k = \cot\theta_k$. Consequently

$$\chi_n(\alpha;\lambda) = \prod_{k=0}^{n-1}\left(\lambda - \cot\frac{\alpha + k\pi}{n}\right). \tag{2.3}$$

□

Remark 2.2. An alternative formula for this polynomial can be found in [20, Formula (4)]. Indeed the coefficients of this polynomial are as follows

$$\begin{aligned} \chi_n(\alpha;\lambda) &= \operatorname{Im}(a+i)(\lambda - i)^n \\ &= \operatorname{Im}\sum_{k=0}^{n}\binom{n}{k}(a+i)\lambda^k(-i)^{n-k} \\ &= \operatorname{Im}\sum_{k=0}^{n}\binom{n}{k}(a(-i)^{n-k} - (-i)^{n-k+1})\lambda^k \\ &= \sum_{k=0}^{n} c_k\lambda^k \end{aligned} \tag{2.4}$$

where

$$c_k = \begin{cases} \binom{n}{k}(-1)^{(n-k)/2} & n-k \text{ even} \\ a\binom{n}{k}(-1)^{(n-k+1)/2} & n-k \text{ odd} \end{cases}$$

or equivalently,

$$c_{n-k} = \binom{n}{k}\left(\cos\frac{k\pi}{2} + a\sin\frac{k\pi}{2}\right) = \begin{cases} \binom{n}{k}(-1)^{k/2} & k \text{ even} \\ a\binom{n}{k}(-1)^{(k+1)/2} & k \text{ odd} \end{cases}$$

cf. [20, Formula (4b)].
In fact the discussion of [20] starts by showing that the characteristic polynomial $\chi_n(\alpha; x)$ is related to the expression $\sin\operatorname{arccot} x$. Indeed evaluation of the polynomial (2.1) at $\lambda = \cot\theta$ and few elementary manipulations yield the identity

$$\chi_n(\alpha; \cot\theta) = \frac{\sin(n\theta - \alpha)}{\sin\alpha \sin^n\theta}.$$

2.2. **Formulas for $\tan(nx)$.** A simple manipulation of the addition formulae for sine and cosine show that the tangent function obeys the addition rule

$$\tan(x + y) = \frac{\tan x + \tan y}{1 - \tan x \tan y} \tag{2.5}$$

This rule is not practical for iteration and the following equivalent elegant formula proposed by Szmulowicz [46] is a convenient alternative

$$\frac{1 + i\tan\sum x_k}{1 - i\tan\sum x_k} = \prod \frac{1 + i\tan x_k}{1 - i\tan x_k} \tag{2.6}$$

It follows immediately from the identity

$$e^{2ix} = \frac{1 + i\tan x}{1 - i\tan x} \tag{2.7}$$

and in particular, $\tan(n \arctan z)$ is a rational function. Indeed

$$\frac{1 + i\tan(nx)}{1 - i\tan(nx)} = \left(\frac{1 + i\tan x}{1 - i\tan x}\right)^n \tag{2.8}$$

and thus

$$\tan(nx) = i\frac{1 - \left(\frac{1+i\tan x}{1-i\tan x}\right)^n}{1 + \left(\frac{1+i\tan x}{1-i\tan x}\right)^n} \tag{2.9}$$

$$= i\frac{(1 - i\tan x)^n - (1 + i\tan x)^n}{(1 - i\tan x)^n + (1 + i\tan x)^n} \tag{2.10}$$

and

$$\cot(nx) = i\frac{(\cot x + i)^n + (\cot x - i)^n}{(\cot x + i)^n - (\cot x - i)^n}. \tag{2.11}$$

Thus we obtain the well known formula [5, item 16]

$$\tan(n \arctan z) = i\frac{(1 - iz)^n - (1 + iz)^n}{(1 - iz)^n + (1 + iz)^n}; \tag{2.12}$$

comparing with the reciprocal polynomial of (2.1) at $a = \cot\alpha = 0$ which is

$$\tilde{p}_n(z) = z^n \chi_n(0; 1/z) = \frac{(1 - iz)^n + (1 + iz)^n}{2}$$

we see that

$$\tan(n \arctan z) = -\frac{1}{n+1}\frac{\tilde{p}'_{n+1}(z)}{\tilde{p}_n(z)}. \tag{2.13}$$

2.3. **Formulas for** $\tan(nx - \alpha)$**.** In view of later applications we introduce a nonzero offset into equation (2.8) and obtain

$$\frac{1 + i\tan(nx + \alpha)}{1 - i\tan(nx + \alpha)} = \left(\frac{1 + i\tan x}{1 - i\tan x}\right)^n \frac{1 + i\tan\alpha}{1 - i\tan\alpha} \tag{2.14}$$

which after a few manipulations yields the identity

$$\tan(nx + \alpha) = i\frac{1 - \left(\frac{1+i\tan x}{1-i\tan x}\right)^n \frac{\cot\alpha + i}{\cot\alpha - i}}{1 + \left(\frac{1+i\tan x}{1-i\tan x}\right)^n \frac{\cot\alpha + i}{\cot\alpha - i}} \tag{2.15}$$

$$= i\frac{(\cot\alpha - i)(1 - iz)^n - (\cot\alpha + i)(1 + iz)^n}{(\cot\alpha - i)(1 - iz)^n + (\cot\alpha + i)(1 + iz)^n} \tag{2.16}$$

The reciprocal provides the following crucial identity for cot

$$\cot(nx - \alpha) = -i\frac{(\cot\alpha + i)(1 - iz)^n + (\cot\alpha - i)(1 + iz)^n}{(\cot\alpha + i)(1 - iz)^n - (\cot\alpha - i)(1 + iz)^n} \tag{2.17}$$

which after comparison with the reciprocal polynomial

$$\tilde{\chi}_n(\alpha; z) = z^n \chi_n(\alpha; 1/z) = \frac{(\cot\alpha + i)(1 - iz)^n - (\cot\alpha - i)(1 + iz)^n}{2i}$$

identifies to

$$\cot(n \arctan z - \alpha) = \frac{1}{n+1}\frac{\tilde{\chi}_{n+1}'(\alpha; z)}{\tilde{\chi}_n(\alpha; z)} \tag{2.18}$$

2.4. **Derivatives of** $\tan$ **and** $\cot$**.** The higher derivatives of $\tan z$ and $\cot z$ are closely related, since $\cot z = \tan\left(\frac{\pi}{2} - z\right)$. It is easy to see that there exist polynomials $P_n(z)$ such that $\frac{d^n}{dz^n}\tan z = P_n(\tan z)$; indeed these *derivative polynomials* satisfy the recursion

$$P_{n+1}(x) = (1 + x^2)P_n'(x)$$

and can be used to efficiently compute tangent and Bernoulli numbers [34]. Explicitly, these polynomials can be expressed via the *geometric polynomials* [10, (2.1)]

$$\omega_n(x) = \sum_{k=0}^{n} \left\{ {n \atop k} \right\} k!\, x^k \tag{2.19}$$

as follows, see [10, (3.10–11)]:

$$P_n(z) = (2i)^n (z + i)\,\omega_n\left(-\frac{iz + 1}{2}\right) = (-2i)^n (z - i) \sum_{k=0}^{n} \frac{k!}{2^k} \left\{ {n \atop k} \right\} (iz - 1)^k \tag{2.20}$$

On the other hand (see [1, Lemma 2.1] or [10, (3.15)])

$$\frac{d^n}{dz^n}\cot z = (-1)^n P_n(\cot z) = (2i)^n (\cot z - i) \sum_{k=1}^{n} \frac{k!}{2^k} \left\{ {n \atop k} \right\} (i\cot z - 1)^k \tag{2.21}$$

and thus $(-1)^n P_n(x)$ serve as derivative polynomials for cot.
Interest in these polynomials goes back at least to Ramanujan [7, Chapter 7, entry 11] and there is some literature, see for example [39, 14, 31, 32, 26, 48].

2.5. **Tangent and arctangent numbers.** The *tangent numbers* are the Taylor coefficients of the tangent function. They make up the odd part of the sequence of E_n of *Euler zigzag numbers*, which are given by the exponential generating function

$$\tan(z) + \sec(z) = \sum_{n=0}^{\infty} \frac{E_n}{n!} z^n. \tag{2.22}$$

The higher order tangent numbers [14] are defined as coefficients of the series

$$\tan^k z = \sum_{n=k}^{\infty} \frac{T_n^{(k)}}{n!} z^n; \tag{2.23}$$

Their bivariate generating function

$$\begin{aligned} T(x,z) &= \sum_{k=1}^{\infty} x^k \tan^k z \\ &= \sum_{n=0}^{\infty} \sum_{k=1}^{n} \frac{T_n^{(k)}}{n!} x^k z^n \\ &= \frac{x \tan z}{1 - x \tan z} \\ &= \sum_{n=0}^{\infty} \frac{T_n(x)}{n!} z^n \end{aligned}$$

where $T_n(x) = \sum_{k=1}^{n} T_n^{(k)} x^k$. On the other hand, from the addition formula (2.5) we infer the exponential generating function of the derivative polynomials to be

$$P(x,z) = \sum_{n=0}^{\infty} P_n(x) \frac{z^n}{n!} = \frac{x + \tan z}{1 - x \tan z}. \tag{2.24}$$

Comparing the two generating functions we find the relation

$$x P_n(x) = (1 + x^2) T_n(x). \tag{2.25}$$

On the other hand let us denote by $A_n^{(k)}$ the *arctangent numbers* (see [16, p. 260] or [19]) defined by their exponential generating function

$$\frac{(\arctan z)^k}{k!} = \sum_{n=k}^{\infty} \frac{A_n^{(k)}}{n!} z^n; \tag{2.26}$$

notice that $A_n^{(k)} = 0$ unless $n-k$ is even and that up to sign these are the same as the coefficients of the hyperbolic arctangent function

$$\frac{(\operatorname{atanh} z)^k}{k!} = \sum_{n=k}^{\infty} \frac{\tilde{A}_n^{(k)}}{n!} z^n. \tag{2.27}$$

The latter are nonnegative and

$$A_n^{(k)} = (-i)^k i^n \tilde{A}_n^{(k)}. \tag{2.28}$$

2.6. **Derivatives of** $\arctan$**.** The derivatives of $\arctan z$ are rational functions and it is easy to verify by induction that they are given by the following formulas

$$\frac{d}{dz} \arctan z = \frac{1}{1+z^2} = \frac{1}{2i} \left(\frac{1}{z-i} - \frac{1}{z+i} \right),$$

and thus

$$\frac{d^m}{dz^m} \arctan z = \frac{i(-1)^m (m-1)!}{2} \left((z-i)^{-m} - (z+i)^{-m} \right). \tag{2.29}$$

2.7. **Faà di Bruno's formula.** In this section we briefly recall the combinatorics behind the composition of exponential generating functions. Let $(a_n)_{n\geqslant 1}$ and $(b_n)_{n\geqslant 1}$ be sequences and define a new sequence by their combinatorial convolution

$$c_n = \sum_{\pi\in\mathcal{P}(n)} a_{|\pi|} \prod_{B\in\pi} b_{|B|} \tag{2.30}$$

Then Fa di Bruno's formula [43, Theorem 5.1.4] asserts that their exponential generating functions $F_a(z) = \sum_{k=1}^{\infty} \frac{a_k}{k!} z^k$ and $F_b(z) = \sum_{k=1}^{\infty} \frac{b_k}{k!} z^k$ satisfy the relation

$$F_c(z) = F_b(F_a(z)). \tag{2.31}$$

Equivalently, given smooth functions f and g, the m-th derivative of the composed function is

$$\frac{d^m}{dz^m} f(g(z)) = \sum_{\pi\in\mathcal{P}(m)} f^{(|\pi|)}(g(z)) \prod_{B\in\pi} g^{(|B|)}(z). \tag{2.32}$$

3. Trace formula

In this section we apply the trace method to the matrix constructed in the previous section in order to prove certain properties of the sum (1.1).

Theorem 3.1. *(i) The cotangent sum* (1.1) *can be expressed as*

$$\mathrm{S}(m,n,\alpha) = \operatorname{Tr}\left((\cot\alpha J_n + B_n)^m\right) \tag{3.1}$$

(ii) There are universal integer valued polynomials $p_{m,m-2k}(x)$ with rational coefficients such that the cotangent sum (1.1) *can be expressed as a polynomial of degree m in $\cot\alpha$*

$$\mathrm{S}(m,n,\alpha) = \sum_{0\leqslant k\leqslant \lfloor m/2\rfloor} p_{m,m-2k}(n) \cot^{m-2k}\alpha. \tag{3.2}$$

Moreover, for any $n\in\mathbb{N}$, the coefficients $p_{m,m-2k}(n)$ are positive integers.

Example 3.2. For example, we have[1]

(1) $S(1,n,\alpha) = n\cot\alpha$
(2) $S(2,n,\alpha) = n^2\cot^2\alpha + n^2 - n$
(3) $S(3,n,\alpha) = n^3\cot^3\alpha + (n^3-n)\cot\alpha$
(4) $S(4,n,\alpha) = n^4\cot^4\alpha + \frac{4}{3}(n^4-n^2)\cot^2\alpha + \frac{1}{3}n^4 - \frac{4}{3}n^2 + n$
(5) $S(5,n,\alpha) = n^5\cot^5\alpha + \frac{5}{3}(n^5-n^3)\cot^3\alpha + (\frac{2}{3}n^5 - \frac{5}{3}n^3 + n)\cot\alpha$

It will be apparent from (6.1) later that indeed $S(m,n,\alpha)$ is a rational polynomial of degree m in both n and $\cot\alpha$.

Proof. It is clear that the trace (3.1) is a polynomial of degree at most n in $\cot\alpha$. Moreover since the entries of the matrices J_n and B_n are integers, the coefficients $p_{m,m-2k}(n)$ are integers as well. For positivity, we show that the mixed moments of J_n and B_n are positive. To see this, note that $P_n = \frac{1}{n}J_n$ is a self-adjoint projection of rank 1. It follows that for any matrix C_n the compression $P_nC_nP_n$ lies in the 1-dimensional algebra generated by P_n, more precisely, $P_nC_nP_n = \xi^T C_n\xi P_n$ where $\xi = \frac{1}{\sqrt{n}}(1,1,\dots,1)^T$ spans the image of P_n. For our matrix B_n clearly $\xi^T B_n\xi = \sum b_{ij} = 0$ and by antisymmetry, also for odd powers $\xi^T B_n^k\xi = (-1)^k\xi^T B_n^k\xi = 0$. It follows that any mixed moment

$$\begin{aligned}
\operatorname{Tr}(J_n^{k_1}B_n^{l_1}J_n^{k_2}B_n^{l_2}\cdots J_n^{k_r}B_n^{l_r}) &= n^{k_1+\dots+k_r}\operatorname{Tr}(P_n^{k_1}B_n^{l_1}P_n^{k_2}B_n^{l_2}\cdots P_n^{k_r}B_n^{l_r}) \\
&= n^{k_1+\dots+k_r}\operatorname{Tr}(P_nB_n^{l_1}P_nB_n^{l_2}P_n\cdots P_nB_n^{l_r}P_n) \\
&= n^{k_1+\dots+k_r}\xi^T B_n^{l_1}\xi\xi^T B_n^{l_2}\xi\cdots\xi^T B_n^{l_r}\xi \\
&= \begin{cases} = 0 & \text{if some } l_j \text{ is odd} \\ > 0 & \text{if all } l_j \text{ are even.} \end{cases}
\end{aligned}$$

[1] We note in passing that there is a misprint in the formula for $S_5(q;\xi)$ in [20, p. 154].

□

In particular, $\mathrm{S}(m, n, \alpha)$ evaluates to an integer (natural number) whenever $\cot\alpha$ is an integer (natural number). It was observed in [11] to the surprise of the authors that the sums in the next corollary are integer valued; explicit formulas are computed in Corollary 6.4 below. We will see later that even for noninteger values of $\cot\alpha$ the sum may evaluate to an integer, e.g., for $n = 2$ and $\cot\alpha = \frac{1}{2}$, Lucas numbers appear, see (5.1) below.

Corollary 3.3. *The sums*

$$S(2m-1, n, \pi/4) = \sum_{k=1}^{n} (-1)^k \cot^{2m-1} \frac{(2k-1)\pi}{4n}$$
$$S(2m, n, \pi/4) = \sum_{k=1}^{n} \cot^{2m} \frac{(2k-1)\pi}{4n}$$

can be represented as integer-valued polynomials in n of degrees $2m-1$ and $2m$, respectively.

Proof. Applying Lemma 2.1 to the matrix $\left[\begin{smallmatrix} 1 & 1+i \\ 1-i & 1 \end{smallmatrix}\right]_n$, we obtain its eigenvalues as

$$\lambda_k = \cot\left(\frac{\pi}{4n} + \frac{k}{n}\pi\right), \quad \text{for } k \in \{1, \dots, n\},$$

because $\alpha = \operatorname{arccot}(1) = \frac{\pi}{4}$. Let us show how these are related the sums considered by Byrne and Smith [11]. Indeed the corresponding power sums are

$$\sum_{k=1}^{n} \cot^r\left(\frac{\pi}{4n} + \frac{k}{n}\pi\right) = \sum_{k=1}^{\lfloor n/2 \rfloor} \cot^r\left(\frac{\pi}{4n} + \frac{k}{n}\pi\right) + \sum_{k=\lfloor n/2 \rfloor + 1}^{n} \cot^r\left(\frac{\pi}{4n} + \frac{k}{n}\pi\right)$$

and substituting $\cot(\frac{\pi}{4n} + \frac{k}{n}\pi) = -\cot(-\frac{\pi}{4n} + \frac{n-k}{n}\pi)$ into the second sum, we get

$$= \sum_{k=1}^{\lfloor n/2 \rfloor} \cot^r\left(\frac{\pi}{4n} + \frac{k}{n}\pi\right) + \sum_{k=0}^{n-\lfloor n/2 \rfloor - 1} (-1)^r \cot^r\left(-\frac{\pi}{4n} + \frac{k}{n}\pi\right)$$
$$= \begin{cases} -\sum_{k=1}^{n} (-1)^{k-1} \cot^r \frac{(2k-1)\pi}{4n} & \text{if } r \text{ is odd,} \\ \sum_{k=1}^{n} \cot^r \frac{(2k-1)\pi}{4n} & \text{if } r \text{ is even.} \end{cases}$$

□

Remark 3.4. (1) The second part of Theorem 3.1 could be seen as a very special case the BMV conjecture [41]: if A and B are positive semi-definite matrices, then for all positive integers m, the polynomial in t, $\mathrm{Tr}(A + tB)^m$, has only non-negative coefficients. The proof above shows that the assertion is also true whenever A is an orthogonal projection of rank one and B is a positive or antisymmetric self-adjoint matrix.

(2) From the Newton identities between power sum and elementary symmetric polynomials we conclude

$$\sum_{l_1 < l_2 < \cdots < l_k} \prod_{j=1}^{k} \cot \frac{\alpha + l_j \pi}{n} = (-1)^{-k} c_{n-k} = \begin{cases} \binom{n}{k}(-1)^{-k/2} & k \text{ even} \\ \cot\alpha \binom{n}{k}(-1)^{(1-k)/2} & k \text{ odd.} \end{cases} \tag{3.3}$$

in situation when $|B| = 1$, then we reduce to Theorem 6.1 with $m = 1$ or when For $|B| = n$ this is confirmed by the well known identities

$$\prod_{k=0}^{n-1} \sin\left(\frac{k\pi}{n} + z\right) = 2^{1-n} \sin(nz) \text{ and } \prod_{k=0}^{n-1} \cos\left(\frac{k\pi}{n} + z\right) = 2^{1-n} \sin\left(nz + \frac{\pi}{2}n\right).$$

For other literature about trigonometric multiple cotangent sum similar to those in (3.3), we refer the reader to [8, Section 6] and [50].

4. Generating functions

In the present section we compute the generating function of the cotangent sums (1.1), for fixed n, i.e.,

$$F_n(z,\alpha) = \sum_{m=0}^{\infty} \mathrm{S}(m,n,\alpha) z^m,$$

which is the moment generating function of the matrix $\cot\alpha J_n + B_n$ with respect to the non-normalized trace. Moreover we will compute the moment generating function of the matrix B_n with respect to the nonnormalized trace and with respect to the state ω with density matrix $P_n = \frac{1}{n}J_n$, that is,

$$\omega(C) = \mathrm{Tr}(P_n C) = \frac{1}{n}\sum_{i,j}^{n} c_{ij} = \xi^T C \xi$$

where as above by ξ we denote the unit vector $\xi = \frac{1}{\sqrt{n}}(1,1,\dots,1)^T$ and $C = [c_{i,j}]_{i,j=1}^n \in M_n(\mathbb{C})$. The moment generating functions

$$\begin{aligned} M_{xJ_n+B_n}(z) &= \mathrm{Tr}((I - z(xJ_n + B_n))^{-1}), \\ M_{B_n}(z) &= \mathrm{Tr}((I - zB_n)^{-1}), \end{aligned}$$

with respect to the trace are easy to compute directly through the characteristic polynomials. On the other hand, direct computation of

$$\tilde{M}_{B_n}(z) = \omega((I - zB_n)^{-1}) = \mathrm{Tr}(P_n(I - zB_n)^{-1})$$

requires information about the eigenvectors which we could not obtain. It will therefore be computed indirectly. The tangent function and its inverse will play a major role in these computations and we collect some facts about these functions first.

4.1. Generating function for cotangent sums.

Proposition 4.1. *For fixed n the ordinary generating function of the cotangent sums* (1.1) *is*

$$F_n(z,\alpha) = \sum_{m=0}^{\infty}\sum_{k=0}^{n-1} \cot^m \frac{\alpha + k\pi}{n} z^m \tag{4.1}$$

$$= \sum_{k=0}^{n-1} \frac{1}{1 - z\cot\theta_k} \tag{4.2}$$

$$= \frac{n}{1+z^2}(1 - z\cot(n\arctan z - \alpha)) \tag{4.3}$$

where $\theta_k = \frac{\alpha+k\pi}{n}$. More generally, the moment generating function of the matrix pencil $xJ_n + B_n$ is

$$M_{xJ_n+B_n}(z) = \frac{n}{1+z^2}\left(1 + z\frac{x + \tan(n\arctan z)}{1 - x\tan(n\arctan z)}\right). \tag{4.4}$$

Proof. Once we have realized $\cot\theta_k$ as roots of a polynomial, it is easy to write down the generating function of the sequence (1.1) as a logarithmic derivative. Indeed, let

$$\begin{aligned} g_n(z) &= \sum_{k=0}^{n-1} \frac{1}{z - \cot\theta_k} \\ &= \frac{\chi_n'(\alpha;z)}{\chi_n(\alpha;z)} \\ &= n\frac{(\cot\alpha + i)(z-i)^{n-1} - (\cot\alpha - i)(z+i)^{n-1}}{(\cot\alpha + i)(z-i)^n - (\cot\alpha - i)(z+i)^n} \end{aligned}$$

then the ordinary generating function is

$$\begin{aligned}
F_n(z,\alpha) &= \frac{1}{z} g_n\left(\frac{1}{z}\right) \\
&= n\frac{(\cot\alpha+i)(1-iz)^{n-1}-(\cot\alpha-i)(1+iz)^{n-1}}{(\cot\alpha+i)(1-iz)^{n}-(\cot\alpha-i)(1+iz)^{n}} \\
&= \frac{n}{1+z^2}\frac{(\cot\alpha+i)(1-iz)^{n}(1+iz)-(\cot\alpha-i)(1+iz)^{n}(1-iz)}{(\cot\alpha+i)(1-iz)^{n}-(\cot\alpha-i)(1+iz)^{n}} \\
&= \frac{n}{1+z^2}\left(1+iz\frac{(\cot\alpha+i)(1-iz)^{n}+(\cot\alpha-i)(1+iz)^{n}}{(\cot\alpha+i)(1-iz)^{n}-(\cot\alpha-i)(1+iz)^{n}}\right) \\
&= \frac{n}{1+z^2}\left(1-z\cot(n\arctan z-\alpha)\right)
\end{aligned}$$

where in the last step we used identity (2.17). The general formula (4.4) follows by substituting $\alpha = \operatorname{arccot} x$ and the addition formula for tangent (2.5). □

Remark 4.2. In the cases $\alpha = 0$ ($\alpha = \pi/2$, resp.) formula (4.3) reproduces [15, Formula (A7.2) (resp. (C6.2))]. At a first glance for $\alpha = 0$ the sum diverges: $\sum_{k=0}^{n-1} \cot^m \frac{k\pi}{n} = \pm\infty$. However [15, Formula (A7.1)] the sum starts at $k = 1$, i.e., $\sum_{k=1}^{n-1} \cot^m \frac{k\pi}{n}$. Inspection of the partial fraction expansion of the generating function (4.2) however reveals that the term $\frac{1}{1-z\cot\theta_0}$ vanishes as θ goes to zero and the generating function becomes

$$F_n(z,0) = \sum_{k=1}^{n-1} \frac{1}{1-z\cot\theta_k}$$

and this is indeed the generating function of the sums $\sum_{k=1}^{n-1} \cot^m \frac{k\pi}{n}$. In the case $\alpha = \pi/2$ formula (4.3) reproduces [15, Formula (C6.2)]. Indeed, since $\cot(\alpha - \pi/2) = -\tan\alpha$ we have $M_{B_n}(z) = \operatorname{Tr}((I - zB_n)^{-1}) = \frac{n(1+z\tan(n\arctan z))}{1+z^2}$.

4.2. **A functional relation.** In this section we indicate an algorithm to calculate the coefficients $p_{m,m-2k}(n)$, which is the main contribution of this paper. The following lemma is a special case of cyclic Boolean convolution [36]; we reproduce the calculation here for the reader's convenience.

Lemma 4.3. *The generating functions $F_n(z,\alpha)$ and $\tilde{M}_B(z)$ satisfy the relation*

$$M_{xJ_n+B_n}(z) = \frac{nxz\frac{d}{dz}z\tilde{M}_{B_n}(z)}{1-nxz\tilde{M}_{B_n}(z)} + M_{B_n}(z) \tag{4.5}$$

Proof. The first terms of the power series are easy to calculate

$$M_{xJ_n+B_n}(z) = n + xnz + \sum_{m\geqslant 2} \operatorname{Tr}((xJ_n+B_n)^m)z^m \tag{4.6}$$

and for $m \geqslant 2$ we expand the powers and arrange the resulting words according to the last letter:

$$\begin{aligned}
\operatorname{Tr}((xJ_n+B_n)^m) &= \operatorname{Tr}\Big((xJ_n)^m + B_n^m \\
&\quad + \sum_{\substack{k\geqslant 1\\ p_0\geqslant 0\\ p_1,p_2,\dots,p_k\geqslant 1\\ q_1,q_2,\dots,q_k\geqslant 1\\ p_0+q_1+p_1+\dots+q_k+p_k=m}} B_n^{p_0}(xJ_n)^{q_1}B_n^{p_1}(xJ_n)^{q_2}B_n^{p_2}\cdots(xJ_n)^{q_k}B_n^{p_k} \\
&\quad + \sum_{\substack{k\geqslant 1\\ q_0\geqslant 0\\ p_1,p_2,\dots,p_k\geqslant 1\\ q_1,q_2,\dots,q_k\geqslant 1\\ q_0+p_1+q_1+\dots+p_k+q_k=m}} (xJ_n)^{q_0}B_n^{p_1}(xJ_n)^{q_1}B_n^{p_2}(xJ)^{q_2}\cdots B_n^{p_k}(xJ_n)^{q_k}\Big) \\
&= \operatorname{Tr}(B_n^m) + \operatorname{Tr}((xJ_n)^m) \\
&\quad + \sum_{\substack{k\geqslant 1\\ p_0\geqslant 0\\ p_1,p_2,\dots,p_k\geqslant 1\\ q_1,q_2,\dots,q_k\geqslant 1\\ p_0+q_1+p_1+\dots+q_k+p_k=m}} (xn)^{q_1+q_2+\dots+q_k}\operatorname{Tr}(PB_n^{p_1})\operatorname{Tr}(PB_n^{p_2})\cdots\operatorname{Tr}(PB_n^{p_{k-1}})\operatorname{Tr}(PB_n^{p_k+p_0}) \\
&\quad + \sum_{\substack{k\geqslant 1\\ q_0\geqslant 0\\ p_1,p_2,\dots,p_k\geqslant 1\\ q_1,q_2,\dots,q_k\geqslant 1\\ q_0+p_1+q_1+\dots+p_k+q_k=m}} (xn)^{q_0+q_1+\dots+q_k}\operatorname{Tr}(PB_n^{p_1})\operatorname{Tr}(PB_n^{p_2})\cdots\operatorname{Tr}(PB_n^{p_k})
\end{aligned}$$

Inserting this expansion into (4.6) we obtain

$$\begin{aligned}
M_{xJ_n+B_n}(z) &= n + nxz + \sum_{m\geqslant 2}\operatorname{Tr}(B_n^m)z^m + \sum_{m\geqslant 2}(nxz)^m \\
&\quad + \sum_{k\geqslant 1}\left(\frac{xnz}{1-xnz}\right)^k(\tilde{M}_{B_n}(z)-1)^{k-1}\hat{M}_{B_n}(z) \\
&\quad + \frac{1}{1-xnz}\sum_{k\geqslant 1}\left(\frac{xnz}{1-xnz}\right)^k(\tilde{M}_{B_n}(z)-1)^k \\
&= \operatorname{Tr}((I-zB_n)^{-1}) + \frac{nxz}{1-nxz} \\
&\quad + \frac{nxz}{1-nxz}\frac{1}{1-\frac{nxz}{1-nxz}(\tilde{M}_{B_n}(z)-1)}\hat{M}_{B_n}(z) + \frac{1}{1-nxz}\left(\frac{1}{1-\frac{nxz}{1-nxz}(\tilde{M}_{B_n}(z)-1)}-1\right) \\
&= M_{B_n}(z) + \frac{nxz}{1-nxz} + \frac{nxz\hat{M}_{B_n}(z)}{1-nxz\tilde{M}_{B_n}(z)} + \frac{1}{1-nxz\tilde{M}_{B_n}(z)} - \frac{1}{1-nxz} \\
&= M_{B_n}(z) + \frac{1+nxz\hat{M}_{B_n}(z)}{1-nxz\tilde{M}_{B_n}(z)} - 1 \\
&= M_{B_n}(z) + \frac{nxz(\hat{M}_{B_n}(z)+\tilde{M}_{B_n}(z))}{1-nxz\tilde{M}_{B_n}(z)}
\end{aligned}$$

where

$$\begin{aligned}\hat{M}_{B_n}(z) &= \sum_{p_0\geqslant 0, p\geqslant 1} \mathrm{Tr}(PB_n^{p_0+p})z^{p_0+p} \\ &= \sum_{m=1}^{\infty} \sum_{\substack{p_0\geqslant 0\\ p\geqslant 1\\ p_0+p=m}} \mathrm{Tr}(PB_n^m)z^m \\ &= \sum_{m=1}^{\infty} m\,\mathrm{Tr}(PB_n^m)z^m \\ &= z\frac{d}{dz}\tilde{M}_{B_n}(z)\end{aligned}$$

□

Lemma 4.4. *For any x the differential equation*

$$\frac{nxzg'(z)}{1-nxg(z)} + M_{B_n}(z) = M_{xJ_n+B_n}(z) \tag{4.7}$$

with initial condition $g(0) = 1$ has unique solution $g(z) = z\tilde{M}_{B_n}(z) = \frac{1}{n}\tan(n\arctan z)$.

Proof. Observe that the considered expression can be rewritten to the first order linear equations on the standard form

$$g'(z) + q(z)g(z) = p(z).$$

The method involves construction of an explicit solution to show that the associated integral equation has unique solution. So if we substitute $g(z) = \frac{\tan(n\arctan z)}{n}$ we see that this function satisfy equation from Lemma 4.4. □

5. Combinatorial interpretation

In this section we indicate explicit combinatorial interpretations of the coefficients of polynomials (3.2) which express the value of trace of matrices in terms of Dyck paths and rooted binary trees. We emphasize that these coefficients $p_{m,k}(n)$ are nonzero, whenever m and k have the same parity.

5.1. **Dimension 2.** First let us record that for $n = 2$ at offset $\cot\alpha_0 = \frac{1}{2}$ we recover the well known sequence Lucas numbers (A000032 in the encyclopedia of integer sequences [40]). Indeed, the characteristic polynomial (2.1) is

$$\chi_2(\lambda) = \mathrm{Im}(\frac{1}{2}+i)(\lambda-i)^2 = \lambda^2-\lambda-1$$

and the roots are the golden ratios $\phi_\pm = \frac{1\pm\sqrt{5}}{2}$ with moments

$$\mathrm{S}(m,2,\alpha_0) = L_m = \phi_+^m + \phi_-^m \tag{5.1}$$

satisfying the recurrence relation

$$L_m = \begin{cases} 2 & m=0 \\ 1 & m=1 \\ L_{m-1}+L_{m-2} & m\geqslant 2 \end{cases}.$$

5.2. **Interpretation of $\mathrm{Tr}(J_n B_n^{2m})$ in terms of Dyck paths.** For the general case we establish some recurrence relations. An explicit formula will be established in Corollary 6.7 below.

Proposition 5.1. *The moments*

$$d_{n,m} = \mathrm{Tr}(J_n B_n^{2m}) \tag{5.2}$$

satisfy the recurrence

$$\begin{aligned} d_{n,0} &= 1 + d_{n-1,0} = n, \\ d_{1,m} &= \delta_{0,m}, \\ d_{n,m} &= d_{n-1,m} + \sum_{k=0}^{m-1} d_{n-1,k} d_{n,m-k-1}. \end{aligned} \tag{5.3}$$

which is reminiscent of the recurrence relations for the Motzkin numbers.

Proof. The function $Q_n(z) = \frac{\tan(n \arctan z)}{z}$ is rational by (2.13). Indeed $Q_1(z) = 1$ and for higher order the addition theorem for the tangent function (2.5) yields the recurrence

$$Q_n(z) = \frac{1}{z} \tan(\arctan z + (n-1)\arctan z) = \frac{z + \tan((n-1)\arctan z)}{z - z^2 \tan((n-1)\arctan z)} = \frac{1 + Q_{n-1}(z)}{1 - z^2 Q_{n-1}(z)}$$

or eqivalently

$$Q_n(z) = 1 + Q_{n-1}(z) + z^2 Q_{n-1}(z) Q_n(z).$$

From Lemma 4.4 we infer that $\sum_{m=0}^{\infty} d_{n,m} z^{2m} = Q_n(z)$ and we can readily calculate the required recurrence for the moments $d_{n,m}$. □

The continued fraction of the rational function $Q_n(z)$ is finite and was computed in [37]:

$$Q_n(z) = \cfrac{n}{1 - \cfrac{\frac{(n+1)(n-1)}{1\cdot 3} z^2}{1 - \cfrac{\frac{(n+2)(n-2)}{3\cdot 5} z^2}{1 - \cfrac{\frac{(n+3)(n-3)}{5\cdot 7} z^2}{\ddots}}}}$$

We can thus infer from Flajolet's theory of continued fractions [25] the following formula for the moments $d_{n,m}$.

Theorem 5.2.

$$d_{n,m} = n \sum_{\pi \in \mathcal{D}_m} w(\pi) \tag{5.4}$$

where the sum runs over Dyck paths of length at most $2m$ with weights $a_{k-1} = \frac{n-k}{2k-1}$, $b_k = \frac{n+k}{2k+1}$, $k = 1, 2, \ldots, n$.

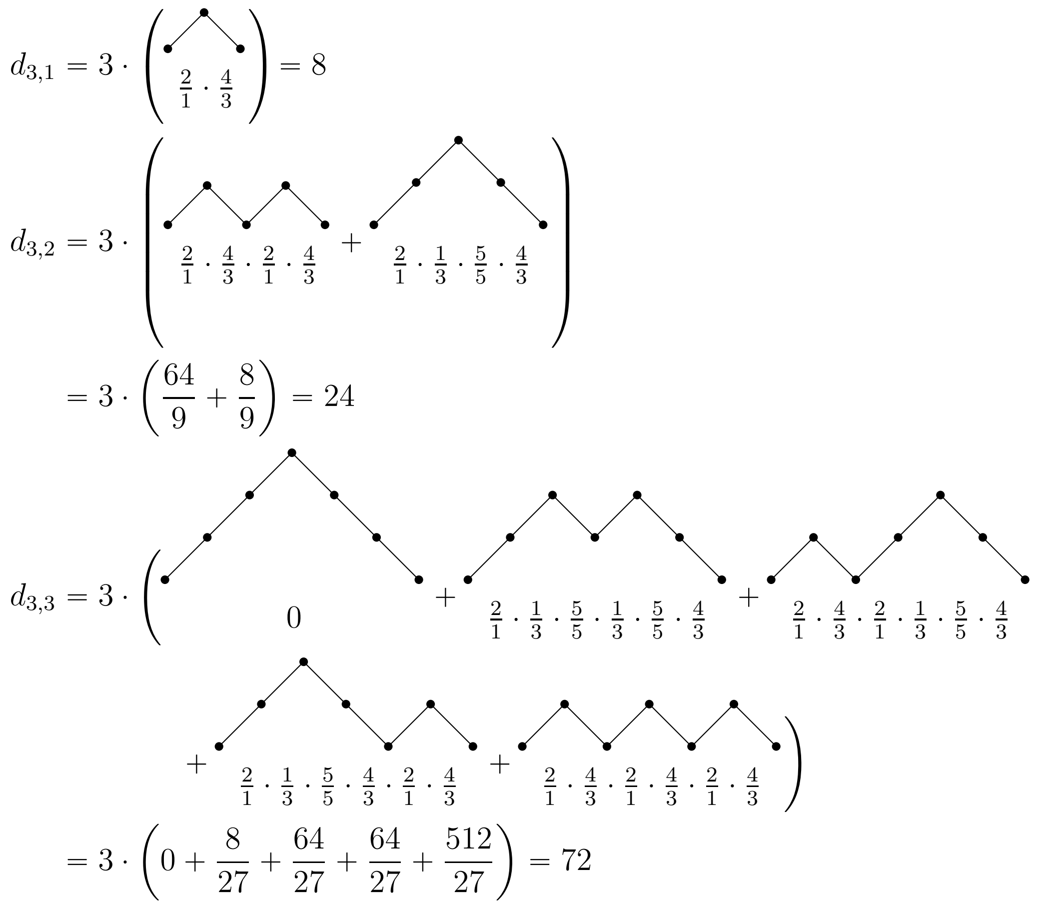
Example 5.3. For $n = 3$ the generating function is

$$Q_3(z) = \frac{z^2 - 3}{3z^2 - 1} = 3 + 8x^2 + 24x^4 + 72x^6 + 216x^8 + 648x^{10} + O\left(x^{11}\right)$$

and indeed for $n = 3$ with weights

$$a_0 = \frac{2}{1}, \quad a_1 = \frac{1}{3}, \quad b_1 = \frac{4}{3}, \quad b_2 = \frac{5}{5}$$

we have



etc.

5.3. **Interpretation of** $\mathrm{Tr}(J_n B_n^{2m})$ **in terms of binary trees.** Set $e_{n,k} = d_{n,k-1}$ and $d_{n,-1} = 1$, then recursion (5.3) can be rewritten more compactly as

$$\begin{aligned} e_{n,0} &= 1, \\ e_{n,1} &= n, \\ e_{1,m} &= \delta_{0,m-1}, \\ e_{n,m} &= \sum_{k=1}^{m} e_{n-1,k} e_{n,m-k}. \end{aligned}$$

which is reminiscent of the Catalan recurrence relations.

Definition 5.4. A *rooted binary tree* is a rooted tree in which each node has at most two children, one of which we distinguish as *firstborn*. We use the convention that the root is not a child and therefore does not count as a firstborn; our trees are unordered but we take the convention that firstborns are always drawn on the right. We denote by $T_{n,m}$ the set of rooted binary trees with m leaves, such that each leaf has a brother and every path emanating from the root contains at most $n-1$ firstborns. We note that the set $T_{n,m}$ is empty unless $m \leqslant n$. For a rooted binary tree $\tau \in T_{n,m}$ we denote by $\mathrm{Paths}(\tau)$ the set of maximal rooted paths. For such a path $p \in \mathrm{Paths}(\tau)$ we denote by $r(p)$ be the number of firstborn nodes occuring in p and its *weight* $\omega(p) = n - r(p)$ which is a number between 1 and n.

Theorem 5.5. *Let* $1 \leqslant m \leqslant n$, *then*

$$e_{n,m} = \sum_{\pi \in T_{n,m}} \prod_{p \in \mathrm{Paths}(\pi)} \omega(p). \tag{5.5}$$

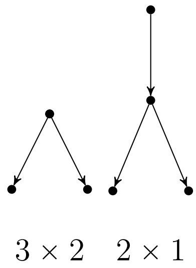


FIGURE 5.1. $T_{3,2}$ with corresponding weight of paths.

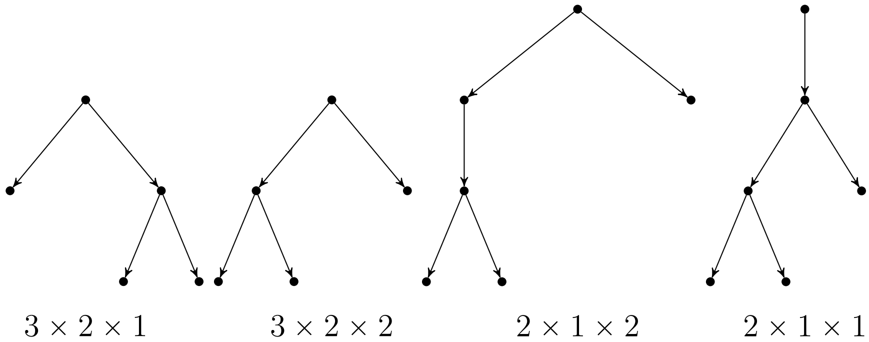
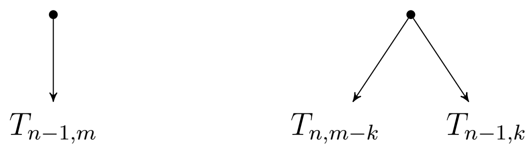


FIGURE 5.2. $T_{3,3}$ with corresponding weight of paths.

Proof. Let us denote the right-hand side of (5.5) by $c_{n,m}$. If $m = 1$ the root is the only node and does not count as a firstborn, therefore $e_{n,1} = c_{n,1} = n$. Moreover $T_{2,2}$ only contains one tree of weight $e_{2,2} = c_{2,2} = 2$. More generally $T_{n,2}$ contains $(n-1)$ trees and $e_{n,2} = c_{n,2} = n(n-1) + (n-1)(n-2) + \cdots + 2 \times 1$. So, it is sufficient to verify that $e_{n,m} = c_{n,m}$ for $n, m \geqslant 3$. Notice that any rooted binary tree can be viewed as one or two (non-empty because $n, m \geqslant 3$) rooted binary trees grafted onto a common root; see Fig. 5.1 and 5.2. Thus in order to create all possible binary trees we start with a root vertex, and one child (Case 1) or two children (Case 2a and 2b) with all possible choices of the subtrees trees as shown in the diagram below.



Case 1. Assume that the root has only one child v_0. Then every path from the root to a leaf with at most $n-1$ firstborns consists of the first step and a path from v_0 with at most $n-2$ firstborns. So the weight remains the same and the number of leaves remains m.
Case 2a). Let τ be such a tree and p a path passing through the firstborn child v_0. Then we can consider the latter as root vertex of new binary tree in $T_{n-1,k}$ with k leaves for $k \in \{1, \ldots, m-1\}$. Denote by p' the restriction of the path p to this subtree. Observe that p' contains at most $n-2$ firstborns because v_0 already counts as a firstborn and the weights of p and p' coincide. Indeed $r(p) = r(p') + 1$ and so $\omega(p) = n - r(p) = n - 1 - r(p') = \omega(p')$.
Case 2b). Let now p be a path passing through the other child, that is, p' is a path in a tree from $T_{n,m-k}$ and again the weight does not change.
Finally we have

$$\sum_{\tau \in T_{n,m}} \prod_{p \in \mathrm{Paths}(\tau)} \omega(p) = \sum_{k=1}^{m-1} \sum_{\tau \in T_{n,m-k}} \prod_{p \in \mathrm{Paths}(\tau)} \omega(p) \sum_{\tau \in T_{n-1,k}} \prod_{p \in \mathrm{Paths}(\tau)} \omega(p) + \sum_{\tau \in T_{n-1,m}} \prod_{p \in \mathrm{Paths}(\tau)} \omega(p),$$

and now we can write

$$c_{n,m} = \sum_{k=1}^{m-1} c_{n-1,k} c_{n,m-k} + c_{n-1,m}$$

Thus we see that $c_{n,m} = e_{n,m}$. □

5.4. **Interpretation of $p_{m,k}(n)$ for $k \geqslant 2$.** The combinatorial objects that we consider now are called circular binary forests.

Definition 5.6. Assume that $m, k \in \mathbb{N}$ have the same parity. For $k \in \{2, \ldots, m\}$ a *circular binary forest* $T^E_{n,m,k}$ of degree k is a set of k binary trees as above arranged on a circle with a total number of m leaves, see Figure 5.3 for an example.

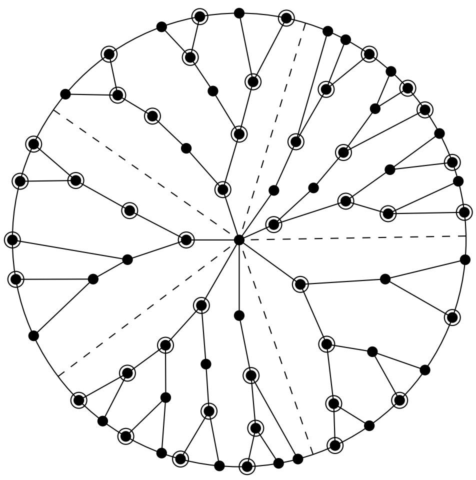


FIGURE 5.3. A circular forest; firstborns are marked with an extra cicle

The *weight* of a forest $F = (\tau_1, \tau_2, \ldots, \tau_k)$ is the product

$$\omega(F) = \prod_{\tau \in F} \omega(\tau).$$

Proposition 5.7. *Assuming that m and k ($k \neq 0$) have the same parity, then*

$$p_{m,k}(n) = \sum_{F \in T^E_{m,n,k}} \omega(F).$$

Proof. From the proof of Theorem (3.1), we see that

$$\begin{aligned} p_{m,k}(n) = & \sum_{\substack{l_0, l_1, \ldots, l_k \geqslant 0 \\ l_1, \ldots, l_{k-1}, l_0 + l_k \text{ even} \\ \sum l_i = m-k}} \mathrm{Tr}(B_n^{l_0} J_n B_n^{l_1} J_n B_n^{l_2} \cdots J_n B_n^{l_k}) \\ & \sum_{\substack{l_0, l_1, \ldots, l_k \geqslant 0 \\ l_1, \ldots, l_{k-1}, l_0 + l_k \text{ even} \\ \sum l_i = m-k}} \mathrm{Tr}(J_n B_n^{l_0 + l_k}) \prod_{1 \leqslant i \leqslant k-1} \mathrm{Tr}(J_n B_n^{l_i}) \end{aligned}$$

This can be visualized in terms of forests, see Figure 5.3. □

5.5. **Interpretation of the constant term $\mathrm{Tr}(B_n^{2m})$.** The moment generating function of B_n is

$$M_{B_n}(z) = \frac{n(1 + z \tan(n \arctan z))}{1 + z^2} = \frac{n + n z^2 Q_n(z)}{1 + z^2}.$$

If we expand the generating function in powers of z, then we obtain

$$\begin{aligned}\operatorname{Tr}(B_n^{2m}) &= nd_{n,m-1} - \operatorname{Tr}(B_n^{2m-2}) = nd_{n,m-1} - nd_{n,m-2} + nd_{n,m-3} + \cdots + nd_{n,0}(-1)^{m-1} + n(-1)^m \\ &= n\sum_{i=0}^{m} d_{n,m-1-i}(-1)^i = n\sum_{i=0}^{m} e_{n,m-i}(-1)^i\end{aligned}$$

6. Explicit analytic evaluation of cotangent sums

In this section we study the Taylor series expansions of the generating function (4.3) and obtain closed formulas in terms of derivative polynomials.

Theorem 6.1. *The cotangent sum* (1.1) *can be expressed as*

$$\mathrm{S}(m,n,\alpha) = (-1)^{m/2} n \mathbb{1}_{m \text{ even}} + \frac{(-i)^m}{(m-1)!} \sum_{\pi\in\mathcal{P}^{odd}(m)} P_{|\pi|-1}(\cot\alpha)(in)^{|\pi|}\mu(\hat{0}_m,\pi) \tag{6.1}$$

where $(-1)^n P_n(x)$ *are the derivative polynomials for* cot (2.21) *and* $\mu(\hat{0}_m,\pi)$ *is the Möbius function of the partition lattice.*

Proof. We start by expressing the generating function (4.3) in terms of the functions $f(z) = \ln(|\sin(z-\alpha)|)$ and $g(z) = n\arctan z$. Indeed observe that

$$\frac{n}{1+z^2}\left(1 - z\cot(n\arctan z - \alpha)\right) = \frac{n}{1+z^2} - z\frac{d}{dz}f(g(z)).$$

and moreover the Leibniz rule of order m implies

$$\frac{d^m}{dz^m}\left(z\frac{d}{dz}f(g(z))\right) = m\frac{d^m}{dz^m}f(g(z)) + z\frac{d^{m+1}}{dz^{m+1}}f(g(z))$$

thus

$$\left.\frac{d^m}{dz^m}\left(z\frac{d}{dz}f(g(z))\right)\right|_{z=0} = \left. m\frac{d^m}{dz^m}f(g(z))\right|_{z=0}.$$

Now we can apply Faà di Bruno's formula (2.32) for the m-th derivative of a composed function and obtain

$$\begin{aligned}\frac{d^m}{dz^m}f(g(z)) &= \sum_{\pi\in\mathcal{P}(m)} f^{(|\pi|)}(g(z)) \prod_{B\in\pi} g^{(|B|)}(z) \\ &= \sum_{\pi\in\mathcal{P}(m)} \cot^{(|\pi|-1)}(g(z)-\alpha) \prod_{B\in\pi} \frac{ni(-1)^{|B|}(|B|-1)!}{2}((z-i)^{-|B|} - (z+i)^{-|B|}) \\ &= \sum_{\pi\in\mathcal{P}(m)} (-1)^{|\pi|-1} P_{|\pi|-1}(\cot(g(z)-\alpha)) \left(-\frac{ni}{2}\right)^{|\pi|} \mu(\hat{0}_m,\pi) \prod_{B\in\pi} ((z-i)^{-|B|} - (z+i)^{-|B|})\end{aligned}$$

where $\mu(\hat{0}_m,\pi) = \prod_{B\in\pi}(-1)^{|B|-1}(|B|-1)!$ is the Möbius function of the partition lattice [42, Example 3.10.4]. Now at $z=0$ we have $g(0)=0$ and

$$(-i)^{-k} - i^{-k} = i^k - (-i)^k = \begin{cases} 0 & k \text{ even} \\ 2i^k & k \text{ odd;} \end{cases}$$

moreover if π is odd then $|\pi| \equiv m \mod 2$ and we obtain

$$\left.\frac{d^m}{dz^m}f(g(z))\right|_{z=0} = -(-i)^m \sum_{\pi\in\mathcal{P}^{\mathrm{odd}}(m)} P_{|\pi|-1}(\cot\alpha)\,(ni)^{|\pi|}\,\mu(\hat{0}_m,\pi) \tag{6.2}$$

finally the Taylor coefficients of $\frac{n}{1+z^2}$ contribute ni^m for even m and the claim follows. □

Corollary 6.2. *The cotangent sums* (1.1) *evaluate to*

$$\mathrm{S}(m,n,\alpha) = (-1)^{m/2} n \mathbb{1}_{m\ even} + \frac{1}{(m-1)!}\sum_{k=1}^{m} n^k A_m^{(k)}\, P_{k-1}(\cot\alpha) \tag{6.3}$$

where $A_m^{(k)}$ *are the arctangent numbers* (2.26)*; note that these are alternating* (2.28)*.*

Proof. We extract the essential part of the formula (6.1) and arrive at the expression

$$\sum_{\pi\in\mathcal{P}^{\mathrm{odd}}(m)} P_{|\pi|-1}(\cot\alpha)(ni)^{|\pi|}\mu(\hat{0}_m,\pi) = \sum_{k=1}^{m} c_{m,k}(ni)^k P_{k-1}(\cot\alpha)$$

where

$$c_{m,k} = \sum_{\substack{\pi\in\mathcal{P}^{\mathrm{odd}}(m)\\ |\pi|=k}} \mu(\hat{0}_m,\pi)$$

This sum can be evaluated using the combinatorial convolution (2.30) by setting

$$f_k = \begin{cases} (k-1)! & \text{for odd } k \\ 0 & \text{else} \end{cases}$$

and $g_k = t^k$ and the generating functions are

$$F_f(z) = \sum_{k\ \mathrm{odd}} \frac{(k-1)!}{k!} z^k = \frac{1}{2}(\log(1+z) - \log(1-z)) = \frac{1}{2}\log\frac{1+z}{1-z} = \operatorname{atanh} z$$

and

$$F_g(z) = \sum_{k=1}^{\infty} \frac{t^k}{k!} z^k = e^{tz} - 1;$$

hence by (2.31)

$$F_g(F_f(z)) = e^{t\operatorname{atanh} z} - 1$$

and the coefficient of t^k yields the desired coefficient $c_{m,k} = \tilde{A}_m^{(k)}$ and from (2.28) we gather the correct sign. □

Remark 6.3. Comtet [16, p. 260] asserts that the arctangent numbers are inverse to the derivative polynomials. This means that the standard monomials can be expanded as a linear combination of tangent polynomials as follows [19, Formula (2.14)]:

$$x^m = \frac{1}{(m-1)!}\sum_{k=1}^{m} A_m^{(k)} P_{k-1}(x) + (-1)^{m/2}\mathbb{1}_{m\ \mathrm{even}} \tag{6.4}$$

Let us explain now that the similarity of this formula with (6.3) is not a coincidence. Indeed using the property that the derivative polynomials linearize the cotangent power and the simple formula $S(1,n,\alpha) = \operatorname{Tr} C_n = n\cot\alpha$ allow for the following alternative straightforward proof:

$$\begin{aligned}
\sum_{s=1}^{n} \cot^m \frac{\alpha+s\pi}{n} &= n(-1)^{m/2}\mathbb{1}_{m \text{ even}} + \frac{1}{(m-1)!}\sum_{s=1}^{n}\sum_{k=1}^{m} A_m^{(k)} P_{k-1}(\cot\frac{\alpha+s\pi}{n}) \\
&= n(-1)^{m/2}\mathbb{1}_{m \text{ even}} + \frac{1}{(m-1)!}\sum_{s=1}^{n}\sum_{k=1}^{m} A_m^{(k)} n^{k-1}(-1)^{k-1}\frac{d^{k-1}}{d\alpha^{k-1}}\cot\frac{\alpha+s\pi}{n} \\
&= n(-1)^{m/2}\mathbb{1}_{m \text{ even}} + \frac{1}{(m-1)!}\sum_{k=1}^{m} A_m^{(k)} n^{k-1}(-1)^{k-1}\frac{d^{k-1}}{d\alpha^{k-1}}\sum_{s=1}^{n}\cot\frac{\alpha+s\pi}{n} \\
&= n(-1)^{m/2}\mathbb{1}_{m \text{ even}} + \frac{1}{(m-1)!}\sum_{k=1}^{m} A_m^{(k)} n^{k-1}(-1)^{k-1}\frac{d^{k-1}}{d\alpha^{k-1}} n\cot\alpha \\
&= n(-1)^{m/2}\mathbb{1}_{m \text{ even}} + \frac{1}{(m-1)!}\sum_{k=1}^{m} A_m^{(k)} n^{k} P_{k-1}(\cot\alpha)
\end{aligned}$$

Let us evaluate formula (6.3) at certain offsets. We start with the elementary evaluations at $\alpha = \pi/2$ and $\alpha = \pi/4$. The first sum vanishes for odd m and yields the free cumulants of the generalized tetilla law, see [24, Proposition 4.10]. The second sum provides an explicit formula for the sums considered by Byrne and Smith [11].

Corollary 6.4.

$$\text{S}(2m, n, \pi/2) = (-1)^m n + \frac{1}{(2m-1)!}\sum_{k=1}^{m} n^{2k} A_{2m}^{(2k)}\, T_{2k-1} \tag{6.5}$$

$$\text{S}(m, n, \pi/4) = (-1)^{m/2} n \mathbb{1}_{m\ even} + \frac{1}{2(m-1)!}\sum_{k=1}^{m} (2n)^{k} A_{m}^{(k)}\, E_{k-1} \tag{6.6}$$

Proof. The evaluation of the generating function (2.24) yields

$$P(0,z) = \tan z \qquad P(1,z) = \frac{1+\tan z}{1-\tan z} = \tan(2z) + \sec(2z)$$

and we conclude that $P_n(0) = T_n$ and $P_n(1) = 2^n E_n = E_n^B$ which are also known as Euler numbers of type B [35]. ☐

Finally let us give an alternative and somewhat simpler expression for the summation formula of Berndt and Yeap [8, Corollary 2.2]

$$\sum_{k=1}^{n-1} \cot^{2m}\frac{k\pi}{n} = (-1)^m n - (-1)^m 2^{2m} \sum_{\substack{j_0,j_1,j_2,\dots,j_{2m}\geqslant 0\\ j_0+j_1+j_2+\dots+j_{2m}=m}} n^{2j_0}\prod_{p=0}^{2m}\frac{B_{2j_p}}{(2j_p)!}.. \tag{6.7}$$

Corollary 6.5. *The sum $S_0(2m,n)$ can be evaluated as follows*

$$\sum_{k=1}^{n-1} \cot^{2m}\frac{k\pi}{n} = (-1)^m (n-1) - \frac{1}{(2m-1)!}\sum_{k=1}^{m}(-1)^k A_{2m}^{(2k)}\frac{4^k B_{2k}}{2k}(n^{2k}-1). \tag{6.8}$$

Proof. The sum $S_0(2m,n)$ can be obtained from the general formula $S(2m,n,\alpha)$ after removing the singular term at $k=0$ and then taking the limit $\alpha \to 0$. Let

$$S_0(2m,n,\alpha) = \sum_{k=1}^{n-1}\cot^{2m}\frac{\alpha+k\pi}{n} = S(2m,n,\alpha) - \cot^{2m}\frac{\alpha}{n},$$

then $S_0(2m,n) = \lim_{\alpha\to 0} S_0(2m,n,\alpha)$. First we linearize the singular term according to formula (6.4) and combine it with the summation formula (6.3) to obtain

$$S_0(2m,n,\alpha) = (-1)^m(n-1) + \frac{1}{(2m-1)!}\sum_{k=1}^{2m} A_m^{(k)}(n^k\, P_{k-1}(\cot\alpha) - P_{k-1}(\cot(\alpha/n))).$$

Next we replace the polynomial evaluation by the derivative according to (2.21) and we see that

$$n^{k+1} P_k(\cot\alpha) - P_k(\cot(\alpha/n)) = (-1)^k (n^{k+1} \cot^{(k)}(\alpha) - \cot^{(k)}(\alpha/n))$$

At this point it is convenient to recall the series expansion of cotangent

$$\cot z = \frac{1}{z} + \sum_{p=1}^{\infty} (-1)^p \frac{2^{2p} B_{2p}}{(2p)!} z^{2p-1}$$

to observe that the derivatives of the singular term $1/z$ cancel and we can express the difference in terms of the analytic part

$$\gamma(z) = \cot z - \frac{1}{z} = \sum_{p=1}^{\infty} (-1)^p \frac{2^{2p} B_{2p}}{(2p)!} z^{2p-1}$$

and find

$$\begin{aligned}
\lim_{\alpha\to 0} n^{k+1} P_k(\cot\alpha) - P_k(\cot(\alpha/n)) &= (-1)^k \lim_{\alpha\to 0} n^{k+1} \gamma^{(k)}(\alpha) - \gamma^{(k)}(\alpha/n)) \\
&= (-1)^k (n^{k+1} - 1) \gamma^{(k)}(0) \\
&= \begin{cases} 0 & k \text{ even} \\ -(-1)^{(k+1)/2} (n^{k+1} - 1) \frac{2^{k+1} B_{k+1}}{k+1} & k \text{ odd} \end{cases}
\end{aligned}$$

and finally

$$\lim_{\alpha\to 0} S_0(2m, n, \alpha) = (-1)^m (n-1) - \frac{1}{(2m-1)!} \sum_{k \text{ even}} (-1)^{k/2} A_m^{(k)} (n^k - 1) \frac{2^k B_k}{k}.$$

□

Remark 6.6. The generating function of the Euler zigzag numbers (2.22) is related to the generating function (2.24)

$$\tan(z) + \sec(z) = \frac{1 + \tan(z/2)}{1 - \tan(z/2)} = \sum_{n=0}^{\infty} P_n(1) \frac{z^n}{2^n n!}$$

and comparing with the explicit formula for the derivative polynomials (2.20) we conclude the following identity:

$$E_n = -(-i)^n \sum_{k=0}^{n} \frac{k!}{2^k} \left\{ {n \atop k} \right\} (i-1)^{k+1}.$$

See [18] for other evaluations of the derivative polynomials at rational angles.

Corollary 6.7. *Extracting the linear coefficient of* (6.3) *we can obtain an explicit expression for the moments* (5.2)

$$\mathrm{Tr}(J_n B_n^{2m}) = \frac{1}{(2m)!} \left(A_{m+1}^{(1)} n + \sum_{k=1}^{2m+1} T_{k-1}^{(2)} A_{2m+1}^{(k)} n^k \right) \tag{6.9}$$

where $T_n^{(k)}$ are the higher tangent numbers (2.23).

7. Concluding Remarks

In this section we connect the algebraic and analytic approach and give some final remarks.

7.1. **Another explicit formula for $\alpha = \frac{\pi}{2}$.** From [28, Problem 76 on P. 317, Answer on P. 559], we infer the identity (cf. [9, (3.29)])

$$\omega_n(-1/2) = \sum_{k=1}^{m} (-1)^k \frac{k!}{2^k} \left\{ {m \atop k} \right\} = \begin{cases} \frac{2}{m+1}(1-2^{m+1})B_{m+1} & \text{if } m \text{ is odd} \\ 0 & \text{if } m \text{ is even.} \end{cases}$$

If we plug in $\alpha = \frac{\pi}{2}$ into Equation (6.1) we will take into account the equation (2.20) then for m even (for m odd the sum is zero) our sums can be written in terms of Bernoulli numbers (which frequently appear in trigonometric sums, see [17, 8, 2, 22, 29])

$$\mathrm{S}(m,n,\pi/2) = (-1)^{m/2} n + \sum_{\substack{\pi \in \mathcal{P}^{\mathrm{odd}}(m) \\ |\pi| \text{ is even}}} \frac{(-1)^{m/2} \pi! (2n)^{|\pi|}}{(m-1)!|\pi|} (1-2^{|\pi|}) B_{|\pi|}.$$

7.2. **Asymptotic analysis and derivative.** In order to investigate asymptotic properties formula from Theorem 6.1 it is sufficient to consider the singleton partition and we obtain

$$\lim_{n\to\infty} \frac{1}{n^m} \sum_{k=0}^{n-1} \cot^m \frac{\alpha + k\pi}{n} = \begin{cases} \frac{1}{(m-1)!} P_{m-1}(\cot\alpha) & \text{if } m > 1 \\ \cot\alpha & \text{if } m = 1. \end{cases}$$

In particular from equation (3.1) we infer the asymptotic expression

$$\frac{1}{(m-1)!} P_{m-1}(z) = \lim_{n\to\infty} \mathrm{Tr}\left[\left(z \begin{bmatrix} 1/n & 1/n \\ 1/n & 1/n \end{bmatrix}_n + \begin{bmatrix} 0 & i/n \\ -i/n & 0 \end{bmatrix}_n \right)^m \right] \quad \text{for } m > 1.$$

Similarly we prove that the derivatives of tangent and cotangent can be approximated by simple matrices.

Finally we examine the limit formula for $\alpha = \frac{\pi}{2}$. From Section 7.1 we conclude

$$\lim_{n\to\infty} \frac{1}{n^m} \sum_{k=0}^{n-1} \cot^m \frac{\frac{\pi}{2} + k\pi}{n} = \begin{cases} \frac{(-1)^{m/2+1} 2^m (2^m - 1) B_m}{m!} & \text{if } m \text{ is even} \\ 0 & \text{if } m \text{ is odd.} \end{cases}$$

Indeed inspecting formula (6.5) immediately yields the asymptotics

$$\sum_{k=0}^{n-1} \cot^{2m}\left(\frac{\pi}{2n} + \frac{k\pi}{n}\right) = (-1)^{m+1} A_{2m}^{(2m)} (2^{2m}-1) n^{2m} \frac{2^{2m} B_{2m}}{(2m)!} + \mathcal{O}(n^{2m-2})$$

and since $A_{2m}^{(2m)} = 1$ this yields the desired limit.

Euler's identity $\zeta(2k) = \frac{(-1)^{k+1}(2\pi)^{2k} B_{2k}}{2(2k)!}$ and above facts leads us to a new approximation of the values of the Riemann zeta function at even integer arguments, namely

$$\zeta(2k) = \lim_{n\to\infty} \frac{\pi^{2k}\, \mathrm{Tr}\left(\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}_n^{2k} \right)}{2n^{2k}(2^{2k}-1)} \quad \text{for } k \in \mathbb{N}.$$

Approximation of the Riemann zeta function for even values by powers of cotangent is well studied, see [47, 3, 21].

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(Wiktor Ejsmont) Instytut Matematyczny, Uniwersytet Wrocławski,, pl. Grunwaldzki 2/4, 50-384 Wrocław, Poland
E-mail address: wiktor.ejsmont@gmial.com

(Franz Lehner) Institut für Diskrete Mathematik, TU Graz Steyrergasse 30, 8010 Graz, Austria
E-mail address: lehner@math.tugraz.at