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Research Paper

A possible positivity of the Li-Keiper coefficients: A general approach based on the Bell polynomials

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ABSTRACT: *We investigate a series related to the Li-Keiper coefficients λn up to n = 1000 and examine the increasing range of positivity of the coefficients using a partition-based approach with Bell polynomials. In particular, the numerical results are compared with the true values, i.e., assuming the truth of the Riemann Hypothesis (RH), and the agreement is very satisfactory. Of greater interest is the emergence of a function, i.e., λn(N), where N is the "order" of the truncation of our decaying alternating series in terms of partitions.*

KEYWORDS*: Li-Keiper coefficients, cluster functions, X partitions, Bell polynomials, numerical experiments, and new equivalence to the Riemann Hypothesis.*

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I. INTRODUCTION

In this work, we continue our analysis of a series that gives the nth Li-Keiper coefficient in terms of the partitions associated to the cluster functions. We briefly recall the results given in [1]. Let λ_n be the Li-Keiper coefficients of the Riemann ξ function, then

$$e^{\sum_{n=1}^{\infty}\lambda_n\frac{z^n}{n}} = \sum_{n=0}^{\infty}\varphi_n z^n \tag{1.1}$$

where φ_n, the cluster functions, are given in [2] as

$$\varphi_n = \sum_{k=0}^{n-1}\frac{1}{(k+1)!}\binom{n-1}{k}\left(\frac{\xi^{(k+1)}(s)}{\xi(s)}\right)\Bigg|_{s=1} \tag{1.2}$$

In [1] the expansion of the λ_n in terms of $\varphi_1,\ldots,\varphi_n$ was analyzed: for example for $n = 1,\ldots,4$ we have

$$\lambda_1 = \varphi_1$$

$$\lambda_2 = 2\varphi_2 - {\varphi_1}^2$$

$$\lambda_3 = 3\varphi_3 - 3\varphi_1\varphi_2 + {\varphi_1}^3$$

$$\lambda_4 = 4\varphi_4 - (4\varphi_1\varphi_3 + 2{\varphi_2}^2) + 4{\varphi_1}^2\varphi_2 - {\varphi_1}^4$$

In [1] we also introduced the notion of blocks: for example λ_4 has 4 blocks

$$4\varphi_4, -4\varphi_1\varphi_3 - 2{\varphi_2}^2, 4{\varphi_1}^2\varphi_2 \ \ and - {\varphi_1}^4$$

all clearly defined (by a specific rule) and having an alternating sign. The rule was heuristically found and will be assessed in the next section.

In the same work, we were also able to obtain the positivity of λ_n up to $n = 30$. Here we continue the analysis of our series up to $n = 1000$, where we confirm the main point i.e. that the range of positivity of the coefficients increases, increasing the number n, whose partitions appear in the indices of the product of the associated cluster functions. The results of the computations for $\lambda_n(N)$ are then compared with the values given by the asymptotic formula assuming the truth of the RH [3] and the agreement is very satisfactory.

II. MAIN IDEA

We illustrate now the idea behind our computations. In Comtet [4] we have the definition of the complete exponential Bell polynomials $B_n(x_1,...,x_n)$ (Y_n in Comtet's book) as

$$e^{\sum_{n=1}^{\infty} x_n \frac{t^n}{n!}} = 1 + \sum_{n=1}^{\infty} B_n(x_1, \dots, x_n) \frac{t^n}{n!} \tag{2.1}$$

Substituting $x_i = (i-1)!\lambda_i$ and $t = z$ in this equation we obtain

$$e^{\sum_{n=1}^{\infty} \lambda_n \frac{z^n}{n}} = 1 + \sum_{n=1}^{\infty} B_n(0!\,\lambda_1, \dots, (n-1)!\,\lambda_n) \frac{z^n}{n!} \tag{2.2}$$

Comparing the RHS of Eq.(2.2) with the RHS of Eq.(1.1) we get

$$n!\,\varphi_n = B_n(0!\,\lambda_1, \dots, (n-1)!\,\lambda_n) \tag{2.3}$$

Now we express λ_n in terms of $\varphi_1,...,\varphi_n$. Still in Comtet [4], the exponential complete Bell polynomials can be expressed as a sum of the exponential partial Bell polynomials as follows

$$B_n(x_1, \dots, x_n) = \sum_{k=1}^{n} B_{n,k}(x_1, \dots, x_{n-k+1}) \tag{2.4}$$

for $n \geq 1$. The exponential partial Bell polynomial are usually defined as

$$B_{n,k}(x_1, \dots, x_{n-k+1}) = \sum \frac{n!}{i_1! i_2! \dots i_{n-k+1}!} \left(\frac{x_1}{1!}\right)^{i_1} \dots \left(\frac{x_{n-k+1}}{(n-k+1)!}\right)^{i_{n-k+1}} \tag{2.5}$$

where the sum runs over $(i_1, i_2, ..., i_{n-k+1})$ such that $i_1 + i_2 + ... + i_{n-k+1} = k$ and $i_1 + 2i_2 + ... + (n-k+1)i_{n-k+1} = n$. Furthermore for the exponential partial Bell polynomials there exists an inverse relation [5]

$$y_n = \sum_{k=1}^{n} B_{n,k}(x_1, \dots, x_{n-k+1}) \tag{2.6}$$

$$x_n = \sum_{k=1}^{n} (-1)^{k-1}(k-1)!\, B_{n,k}(y_1, \dots, y_{n-k+1}) \tag{2.7}$$

which, when applied to our case, yields

$$\lambda_n = \sum_{k=1}^{n} (-1)^{k-1} \frac{(k-1)!}{(n-1)!} B_{n,k}(1!\,\varphi_1, \dots, (n-k+1)!\,\varphi_{n-k+1}) \tag{2.8}$$

The last equation confirms the block structure of the λ_n and corroborates the heuristic rule: both were stated in [1]. Considering now (for $1 \leq N \leq n$)

$$\lambda_n(N) = \sum_{k=1}^{N} (-1)^{k-1} \frac{(k-1)!}{(n-1)!} B_{n,k}(1!\,\varphi_1, \dots, (n-k+1)!\,\varphi_{n-k+1}) \tag{2.9}$$

we look at each $B_{n,k}(.,.)$ polynomial as a "block".

III. COMPUTATIONS

For the computations we use the C library Arb [6], which allow us to compute values with arbitrary precision.

3.1 Asymptotic of the cluster functions φ_n as a function of n

In a previous work we suggested a possible behavior of the cluster functions as a function of *n* given by the inequality

$$\varphi_n > \lambda_1 + cn \ln n$$

We now investigate more carefully the behavior of the cluster functions as a function of *n* by mean of Eq.(1.2). We obtain

n	φ_n	n	φ_n
1	0.0230957089	60	26.4686534118
2	0.0464395735	70	55.9717327028
3	0.0702814218	80	114.7958281665
4	0.0948744358	90	229.3118890120
5	0.1204768473	100	447.6042542058
6	0.1473536597	200	151502.8001800836
7	0.1757784006	300	19836697.2731286423
8	0.2060349167	400	1492739244.8771206717
9	0.2384192163	500	76866613328.6876158273
10	0.2732413707	600	2983019551597.3904557274
20	0.8380155239	700	92684875194748.4009195458
30	2.1810176553	800	2402286130600407.8965011944
40	5.2722701653	900	53493436495315872.8093411454
50	12.0731449939	1000	1046191872311269880.6572978767

Table 1

Note that φ_n seems to build a strictly monotonically increasing sequence as should be for the λ_n's. The first value of φ_n greater than 1 is $\varphi_{22} \approx 1.0226347276$.

On the basis of the results of our actual computations, we can now discard the suggested behavior of the φ_n: it is more plausible, that the values grows $\propto e^{cn}$ for a given constant *c*.

3.2 Analysis of the block sums: some examples of λ_n behavior

Note: All the following tables give values truncated to the tenth decimal place.

Consider $n = 26$

N	$\lambda_{26}(N)$	N	$\lambda_{26}(N)$	N	$\lambda_{26}(N)$
1	39.0957921141	11	14.3178645489	21	14.3178645486
2	1.1179681653	12	14.3178645486	22	14.3178645486
3	17.9091737123	13	14.3178645486	23	14.3178645486
4	13.7210962964	14	14.3178645486	24	14.3178645486
5	14.3845206139	15	14.3178645486	25	14.3178645486
6	14.3125485108	16	14.3178645486	26	14.3178645486
7	14.3181800929	17	14.3178645486		
8	14.3178501855	18	14.3178645486		
9	14.3178650612	19	14.3178645486		
10	14.3178645340	20	14.3178645486		

Table 2

Real value: $\lambda_{26} \approx 14.3178645486$.

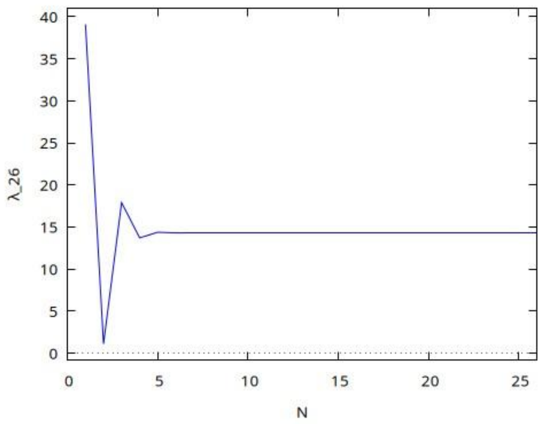

Figure 1: $\lambda_{26}(N)$

Until n = 26 all sums of blocks are positive and there is a clear oscillating behavior, due to the alternation of the sign. Let now n = 27

N	$\lambda_{27}(N)$	N	$\lambda_{27}(N)$	N	$\lambda_{27}(N)$
1	44.6071673430	11	15.3407928666	21	15.3407928657
2	-1.5176080739	12	15.3407928657	22	15.3407928657
3	20.2889690017	13	15.3407928657	23	15.3407928657
4	14.4535855589	14	15.3407928657	24	15.3407928657
5	15.4478234625	15	15.3407928657	25	15.3407928657
6	15.3315606405	16	15.3407928657	26	15.3407928657
7	15.3413865711	17	15.3407928657	27	15.3407928657
8	15.3407635276	18	15.3407928657		
9	15.3407940052	19	15.3407928657		
10	15.3407928304	20	15.3407928657		

Table 3

Real value: $\lambda_{27} \approx 15.3407928657$.

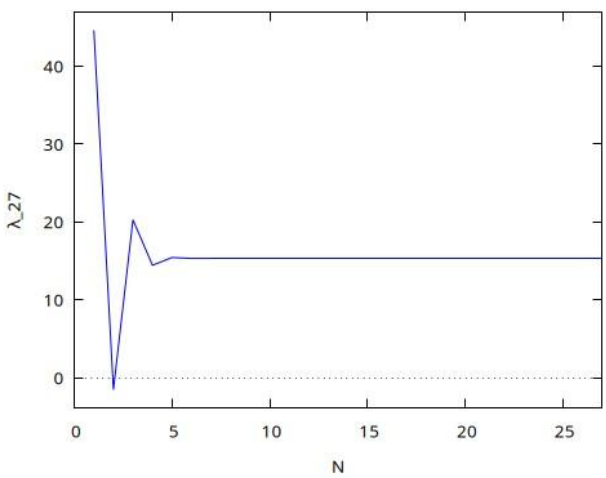

Figure 2: $\lambda_{27}(N)$

By n = 27 we see for the first time a negative sum of blocks: this will appear regularly in the following λ computations. Let now n = 50

N	$\lambda_{50}(N)$	N	$\lambda_{50}(N)$	N	$\lambda_{50}(N)$
1	603.6572496984	21	43.5310964883	41	43.5310964883
2	-1140.1109873199	22	43.5310964883	42	43.5310964883
3	1228.4903746194	23	43.5310964883	43	43.5310964883
4	-672.9385134941	24	43.5310964883	44	43.5310964883
5	336.7563986393	25	43.5310964883	45	43.5310964883
6	-43.3909211668	26	43.5310964883	46	43.5310964883
7	63.0634254326	27	43.5310964883	47	43.5310964883
8	40.0924012823	28	43.5310964883	48	43.5310964883
9	44.0174416491	29	43.5310964883	49	43.5310964883
10	43.4747341407	30	43.5310964883	50	43.5310964883
11	43.5365347474	31	43.5310964883		
12	43.5306538341	32	43.5310964883		
13	43.5311272189	33	43.5310964883		
14	43.5310946518	34	43.5310964883		
15	43.5310965836	35	43.5310964883		
16	43.5310964840	36	43.5310964883		
17	43.5310964885	37	43.5310964883		
18	43.5310964883	38	43.5310964883		
19	43.5310964883	39	43.5310964883		
20	43.5310964883	40	43.5310964883		

Table 4

Real value: $\lambda_{50} \approx 43.5310964883$.

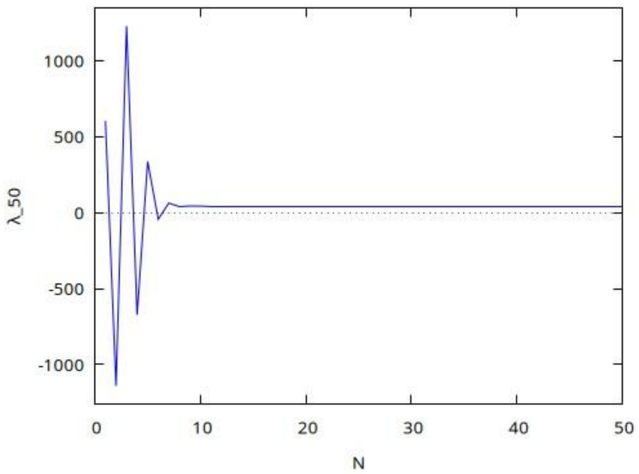

Figure 3: $\lambda_{50}(N)$

A last example for n = 1000: the real value is $\lambda_{1000} \approx 2326.0531616864$. On the plot, the oscillations are undistinguishable.

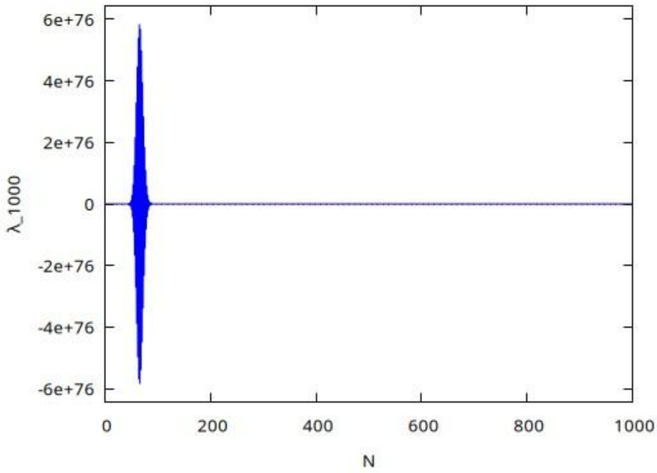

Figure 4: $\lambda_{1000}(N)$

3.3 Analysis of the block sums: negative values

As seen in the previous section, negative block sums only appears when N is even (due to the negative sign). The next table shows the following: given every N even between 2 and 204, for which n the sum in Eq.(2.9) becomes negative for the first time.

N	n	N	n	N	n
2	27	40	214	78	397
4	38	42	224	80	407
6	48	44	234	82	416
8	58	46	243	84	426
10	68	48	253	86	435
12	78	50	263	88	445
14	88	52	272	90	454
16	98	54	282	92	464
18	108	56	291	94	474
20	117	58	301	96	483
22	127	60	311	98	493
24	137	62	320	100	502
26	147	64	330	120	598
28	156	66	339	140	693
30	166	68	349	160	789
32	176	70	359	180	884
34	185	72	368	200	979
36	195	74	378	202	989
38	205	76	387	204	998

Table 5

In Table 5 we see a certain regularity in the slope of the n. This will be more evident in the next table, which contains the gaps between two consecutive values of n (i.e. $\Delta_i = n_{i+1} - n_i$, $i \geq 1$) from Table 5

i	Δ_i	i	Δ_i	i	Δ_i	i	Δ_i
1	11	27	9	53	9	79	10
2	10	28	10	54	10	80	9
3	10	29	10	55	10	81	10

i	Δ_i	i	Δ_i	i	Δ_i	i	Δ_i
4	10	30	9	56	9	82	9
5	10	31	10	57	10	83	10
6	10	32	9	58	9	84	9
7	10	33	10	59	10	85	10
8	10	34	10	60	9	86	9
9	9	35	9	61	10	87	10
10	10	36	10	62	9	88	9
11	10	37	9	63	10	89	10
12	10	38	10	64	9	90	9
13	9	39	10	65	10	91	10
14	10	40	9	66	10	92	9
15	10	41	10	67	9	93	10
16	9	42	9	68	10	94	10
17	10	43	10	69	9	95	9
18	10	44	9	70	10	96	10
19	9	45	10	71	9	97	9
20	10	46	10	72	10	98	10
21	10	47	9	73	9	99	9
22	9	48	10	74	10	100	10
23	10	49	9	75	9	101	9
24	10	50	10	76	10		
25	9	51	9	77	9		
26	10	52	10	78	10		

Table 6

3.3.1 Linear last square fitting

The coefficients m, q of the linear least square fitting ($n = mN + q$) are defined by:

$$\begin{cases} m = \dfrac{\mu_{Nn} - \mu_N \mu_n}{\mu_{N^2} - {\mu_N}^2} \\ q = \mu_{n - m\mu_N} \end{cases}$$

where

$$\mu_N = \frac{1}{r}\sum_{i=1}^{r} N_i \,, \mu_n = \frac{1}{r}\sum_{i=1}^{r} n_{i,} \;\; \mu_{N^2} = \frac{1}{r}\sum_{i=1}^{r} {N_i}^2 \; and \; \mu_{Nn} = \frac{1}{r}\sum_{i=1}^{r} N_i \, n_i$$

Because the N_i are even numbers between 2 and 204 (r = 102)

$$\begin{cases} \mu_N = r + 1 = 103 \\ \mu_{N^2} = \dfrac{2(r+1)(2r+1)}{3} = \dfrac{42230}{3} \end{cases} \Rightarrow \;\; \mu_{N^2} - {\mu_N}^2 = \frac{(r+1)(r-1)}{3} = \frac{10403}{3}$$

The other values are μ_n=8767/17 and μ_{Nn}=3556180/51, resulting in

$$\begin{cases} m = \dfrac{847177}{176851} \approx 4.790343283328904 \\ q = \dfrac{38290}{1717} \approx 22.30052417006408 \end{cases}$$

3.3.2 Lower bound for the *n*

Consider now $d_i = \Delta_i - 9$, that is $d_i \in \{0,1,2\}$. Summing all the d_i from 1 to k yield

$$s_k = \sum_{i=1}^{k} d_i = n_{k+1} - n_1 - 9$$

If we try to approximate $1/s_k$ with $1/k^{\alpha}$ (for a certain α), we have

$$\frac{1}{s_k} < \frac{1}{k^{0.89}} \Rightarrow n_{k+1} > 9(k+3) + k^{0.89}$$

It can be noted, that the difference between n_{k+1} and $9(k+3) + k^{0.89}$ tends towards zero, and it is our opinion, that there will be a $K > 1000$, for which $n_{K+1} < 9(K+3) + K_{0.89}$.

3.3.3 Numerical results vs a probabilistic model

In relation to our numerical results (see Table 6), we remark the following: starting with the 33rd numerical result, the distribution seems to follow a pattern

i	pattern	#9	#10	#11
1	no pattern	9	22	1
33	[10-10]-9-10-9	2	3	0
38	[10-10]-9-10-9-10-9	3	4	0
45	[10-10]-9-10-9-10-9-10-9	4	5	0
54	[10-10]-9-10-9-10-9-10-9-10-9	5	6	0
65	[10-10]-9-10-9-10-9-10-9-10-9-10-9	6	7	0
78	[10-10]-9-10-9-10-9-10-9-10-9-10-9-10-9	7	8	0

Table 7

In the kth pattern 11 appears 0 times, 10 appears $k+2$ times and 9 appears $k+1$ times. Summing the all the occurrences (until the kth pattern)

$$\begin{cases} S_9(k) = 9 + \sum_{j=1}^{k}(j+1) = 9 + \dfrac{k(k+3)}{2} \\ S_{10}(k) = 22 + \sum_{j=1}^{k}(j+2) = 22 + \dfrac{k(k+5)}{2} \\ S_{11}(k) = 1 \end{cases}$$

The total is $S(k) = S_9(k) + S_{10}(k) + S_{11}(k) = 32 + k(k+4)$. That means, that the frequencies (until the kth pattern) are

$$f_9(k) = \frac{k^2+3k+18}{2(k^2+4k+32)}, f_{10}(k) = \frac{k^2+5k+44}{2(k^2+4k+32)}, f_{11}(k) = \frac{1}{k^2+4k+32}$$

and our slope is

$$m = \frac{9f_9(k) + 10f_{10}(k) + 11f_{11}(k)}{2} = \frac{19k^2+77k+624}{4(k^2+4k+32)}$$

The first few values are listed in Table 8

k	m
0	4.875
1	4.864864864864865
2	4.8522727272727275
3	4.839622641509433
4	4.828125
5	4.818181818181818
6	4.809782608695652

Table 8

Note: The case $k = 0$ is the case, where no pattern exists.

Assuming now that the pattern holds when $k \to\infty$, it is easy to see, that

$$\lim_{k\to\infty} f_9(k) = \lim_{k\to\infty} f_{10}(k) = \frac{1}{2} \; and \; \lim_{k\to\infty} f_{11}(k) = 0$$

This means, that our slope is $m \to 19/4=4.75$ (for $k \to\infty$).

IV. OPEN POINTS

Let x_n $(n \geq 1)$ a strictly monotonically increasing sequence and $y_n = B_n(x_1,...,x_n)$ the transformation of the sequence. Under which conditions is y_n $(n \geq 1)$ also a strictly monotonically increasing sequence? For example, we have

x_n	y_n
$(n-1)!$	$n!$
$n!$	$\sum_{k=1}^{n} L(n,k)$
α^n $(\alpha > 1)$	$\alpha^n \sum_{k=1}^{n} \left\{ {n \atop k} \right\} = B_n$
n	$\sum_{k=1}^{n} \binom{n}{k} k^{n-k}$

where $L(n,k)$ are the Lah numbers, $\left\{ {n \atop k} \right\}$ are the Stirling numbers of the second kind and B_n are the Bell numbers.

Conjecture 4.1 (Monotonicity of Bell polynomials summations)**.** *Let I_1 be a class of strictly monotonically increasing sequences with certain properties and I_2 another class of strictly monotonically increasing sequences with other properties. Let x_n and y_n $(n \geq 1)$ be two strictly monotonically increasing sequences with*

$$y_n = \sum_{k=1}^{n} B_{n,k}(x_1, \dots, x_{n-k+1})$$

$$x_n = \sum_{k=1}^{n} (-1)^{k-1}(k-1)!\, B_{n,k}(y_1, \dots, y_{n-k+1})$$

Then, $x_n \in I_1 \Longleftrightarrow y_n \in I_2$.

Conjecture 4.2. *Let φ_n the sequence of the cluster functions defined by (1.2), then, under Conjecture* 4.1*, the Riemann Hypothesis is equivalent to* $0 < \varphi_1 < \dots < \varphi_n < \varphi_{n+1} < \dots$.

V. CONCLUSION

By means of the partial Bell polynomials the experiment up to $n = 1000$, with the approach of the block's partitions, we have found that:

- The range of positivity of λ_n increases with n: employing more quantitative amounts of the k-partitions blocks in terms of the φ's (i.e. truncation up to N) the set of values obtained converge to the true values.
- The above approach do not make uses of the set of the nontrivial zeros of the ζ function and is merely connected with a counting procedure [7, 8] i.e., a combinatorics with the partitions [9, 10, 11] in the indices of the blocks of the cluster functions.

- The presence of negatives sums in the alternating behavior of the $\lambda_n(N)$, whose index N slowly increases but seems never to reach n (see the slope in Subsection 3.3.3), does not affect the convergence of the whole sum Eq.(2.8) to the real value of λ_n.

To the best of our knowledge, the approach and computations above are new or have not been obtained along these lines, and they provide a new equivalent of the RH using rigorous Bell polynomial methods.

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