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Review Paper

Thermodynamic limit for the low Li-Keiper coefficients: upper and lower bounds

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Abstract
We consider the set of the first 6 Equations relating a spin ½ system with long-range ferromagnetic interaction on a circle with a truncation of the Riemann Xi function.
We explicitly give the values of the first 6 Li-Keiper coefficients in the thermodynamic limit as functions of the first one i.e. $\lambda_1 = (1+\gamma/2-(1/2)\cdot\log(4\cdot\pi) = 0.0230957...$
We then report the results, i.e., a numerical Table and plots both, with upper and lower bounds (2N→□) for the true values of λ_n*, n = 1, .., 6.*
Keywords: *Li-Keiper coefficients, Ferromagnetic Spin ½ model, thermodynamic limit (2N→□), stability, Bounds, Locus of Zeros, Riemann Hypothesis (RH).*

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I. Introduction

In this note, related to some recent our works [1, 2] we start with a set of Equations for a spin ½ system on a dodecagon (2N=12 spins on a circle) with a magnetic field variable $z = e^{(-2\cdot\beta H)}$, a two-body ferromagnetic interaction $e^{(-2\cdot\beta J)}$, and the related truncation of the Riemann ξ function in the variable z=1-1/s with s the usual complex number, i.e. s=Re(s)+i·Im(s) = ρ+i·t.
The set of Equations of interest here is given by [1, 2]:
(φ_0=1)

$$\binom{2N}{i}\cdot X^{i\cdot(2N-i)} = \sum_{k=0}^{i}\binom{2N}{i-k}\cdot(-1)^k\cdot\varphi_k \tag{1}$$

where φ_k is the cluster function of order k, i.e. a function of the Li-Keiper coefficients λ_p for p from 1 to k.
We notice that $\varphi_1 = \lambda_1$; the first two above Equations read:

$$2\cdot N\cdot X^{(2N-1)} = 2\cdot N - \varphi_1 = 2\cdot N - \lambda_1 \tag{2}$$

and

$$\binom{2N}{2}\cdot X^{2\cdot(2N-2)} = \binom{2N}{2} - 2N\cdot\varphi_1 + \varphi_2 \tag{3}$$

where $\varphi_2 = (½)\cdot(\lambda_2 + \lambda_1^2)$.

We now add that if we are interested in studying the true dodecagon i.e. 2N=12 we have the 6 Equations which give us the first 6 values of the Li-Keiper coefficients for the dodecagon, values which (as for the hexagon already treated in [3]) are below the true values, i.e. we obtain: λ_n (2N=12), n=1..6.
We illustrate here the situation only with the computation of λ_2.

In fact with X= $e^{(-2\cdot\beta\cdot J)}$, given by Eq.(2), inserted in Eq.(3), we obtain for 2N=12:

$$\varphi_2 = \frac{2N\cdot(2N-1)}{2}\cdot\left(\left(1-\frac{\lambda_1}{2N}\right)^{2\cdot(2N-2)/(2N-1)} - 1\right) + 2N\cdot\lambda_1 = \quad (4)$$

$$= 66\cdot\left(\left(1-\frac{\lambda_1}{12}\right)^{\frac{20}{11}} - 1\right) + 12\cdot\lambda_1 = 0.04637329$$

with λ_1 =1+γ/2 -(1/2)·log(4·π) we obtain values near and smaller than the true values, for n=1..6, on Table 1.

λ_2	$= 2.\varphi_2 - \lambda_1^2 = 0.092213168 < 0.0923457..$
λ_3	$= 0.206846937 < 0.207638920..$
λ_4	$= 0.366150325 < 0.368790479...$
λ_5	$= 0.568965028 < 0.575542714...$
λ_6	$= 0.8138172484 < 0.827566012$

Table 1.

II. The thermodynamic limit

We are now merely interested in the thermodynamic limit 2N→∞, (i.e., we forget now the dodecagon and we consider an infinite spin system as well as an infinite truncation of the series for the ξ function), and this up to n = 6.
We obtain in this way an upper bound to λ_n, for n=1..6.
In fact, Eq.(4) gives as 2N→∞:

$$\varphi_2 = 2\cdot\lambda_1 + \lambda_1^2/2 + O(1/2\cdot N)$$

thus:

$$\lambda_2^* = 2\cdot\varphi_2 - \lambda_1^2 = 4\cdot\lambda_1 = 0.092382836.. > 0.0923457..$$

i.e. we obtain a value λ_2^* greater than the true value λ_2 = 0.0923457..

Moreover from early finding [4] we have some kind of "stability" (in the sense of statistical Mechanics) in that we also have a lower bound given by the first value emerging from our Riemann wave background [1, 2] i.e. that related to the smallest spin system (2N=2, stability) and given by: $\lambda'_2 = 4\cdot\lambda_1 - \lambda_1^2 = 0.09184942..$

Below, we report the corresponding Table 2 of values for the upper bounds λ^*_n (given by $\lambda^*_n = n^2\cdot\lambda_1$, see Appendix for the proof), the true values λ_n and the lower bounds λ'_n offered by Riemann wave background for n =1 to n=6.

n	**λ'_n**	**λ_n**	**λ^*_n**
1	0.02309570	0.02309570	0.02309570
2	0.09184942	0.09234573	0.09238283
3	0.20467322	0.20763892	0.20786138
4	0.35896136	0.36879047	0.36953134
5	0.55115045	0.57554271	0.57739272
6	0.77680175	0.82756601	0.83144552

Table 2. The lower bounds λ'_n, the true values λ_n, and the upper bounds $\lambda^*_n = n^2\,\lambda_1$, n=1..6.

III. Locus of Zeros for 2N up to 56 (unit circle versus critical line)

In this Section we analyze the following point: the spin model as presented, is limited to some values of the number $2\cdot N$, i.e. the number of spin variables on the circle. In fact, the values of the Li-Keiper coefficients which follow are given by:

$\lambda_n (2\cdot N \to \infty) = n^2\cdot\lambda_1 = n^2\cdot (1+\gamma/2-(1/2)\cdot\log(4\cdot\pi) = n^2\cdot 0.0230957\ldots$
(See appendix for the proof).
We add here that with the truncation, λ_1 should be a function of N, i.e. a better approximation for the Li-Keiper coefficients.
This may be seen by the product formula in the definition of the ξ function in term of the zeros i.e. by:

$$\xi(s) = \xi(1-s) = \prod_{\rho}\left(1-\frac{(1-s)}{\rho}\right)$$

where $s=\mathrm{Re}(s)+i\cdot\mathrm{Im}(s)$.

Introducing the variable $z=1-1/s$ or $s=1/(1-z)$, then

$1-(1-s)/\rho = 1-(1-1/(1-z))/\rho = 1+z/[(1-z)\cdot\rho]$

$$\xi(s) = e^{\left\{ln\left[\prod_{\rho}\left(1+\frac{z}{(1-z)\cdot\rho}\right)\right]\right\}}$$

$z\sim 0$ ($s\sim 1$); then with the Taylor expansion:

$$\xi(1-s) = e^{\sum_{\rho}\ln\left(1+\frac{z}{(1-z)\cdot\rho}\right)} = e^{\sum_{\rho}\left(\frac{z}{(1-z)\cdot\rho}-\frac{1}{2}\frac{z^2}{\cdot(1-z)^2\cdot\rho^2}+\cdots\right)} =$$

$$= e^{\sum_{\rho}\left(\frac{z}{\rho}+\frac{z^2}{\rho}-\frac{1}{2}\frac{z^2}{\rho^2}\cdots\right)} =$$

$$= e^{\left(z\cdot\sum_{\rho}\frac{1}{\rho}+\frac{z^2}{2}\cdot\sum_{\rho}\left(\frac{2}{\rho}-\frac{1}{\rho^2}\right)+\cdots\right)} =$$

$$= e^{\left(z\cdot\lambda_1+\frac{z^2}{2}\lambda_2+\cdots\right)}$$

Since we have considered a truncation, then (for a spin system of 2N spins variables) we have N zeros above t=0.
We then introduce in the formulas not λ_1 but λ_1* solution of the next Equation.

$N(t) = (t/2\pi)\cdot(\ln(t/2\pi) -1) +7/8 +(1/\pi)\cdot\mathrm{argument}(\zeta(1/2+i\cdot t)$
in the approximation $N(t) = (t/2\pi)\cdot(\ln(t/2\pi) -1) + 7/8$, where the solution is given in terms of the Lambert W function [5] by:

$$t = f(N) = 2\cdot\pi\cdot e^1\cdot e^{\left(W\cdot\left(\frac{N-\frac{7}{8}}{e^1}\right)\right)}$$

Then:

$$\lambda_1^* = f(N) = \sum_{k=41}^{k=N}\frac{1}{\left(t^2\,(k)+\frac{1}{4}\right)} + 0.0170313299451 \tag{5}$$

where the last number is the contribution of the first 40 zeros of $\zeta(1/2+i\cdot t)$ [6]. The result is given in the Figure 1.

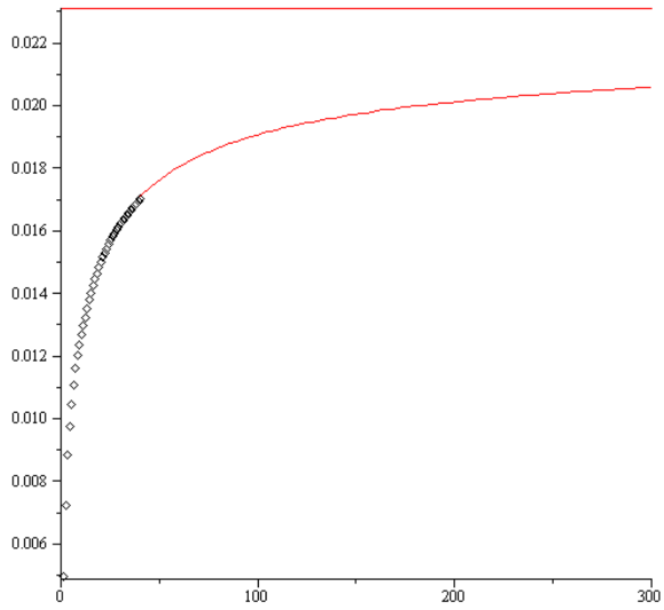

Fig. 1. Point plot of f(N) from N=1 to N=40 (in black) and f(N) by means of the LambertW function i.e. Eq. (5), N>40.

We now analyze the relation between n and N i.e. we look at the solution of the Equation: $n^2\cdot\lambda_1^*(N)=\lambda_n$, in order to see, for a given N, what n's are allowed with $\lambda_1^* < \lambda_n/n^2$. As an example, for n=2, $\lambda_2/4 = 0.0923457/4 = 0.023086425$ and we obtain f(N) = 0.023086425 i.e. n < 50000.
For N=28, we have f(28)=0.016128926 and for this value Eq. (5) above gives n<29.This means that with a system of 2.28=56 spins, the thermodynamic limit gives a value of the first 28 lambda's near and still smaller than the true value λ_n and from our construction (i.e. the meeting of the spin model with magnetic field variable $z=e^{(-2\cdot\beta\cdot H)}$ with the truncation of the function in the variable z) the 56 degree polynomial in z of the truncated function $\xi(z)$, has all its zeros in z on the unit circle (Lee-Yang theorem) and thus all the zeros in s= 1/(1-z) on the critical line).

Remark
The upper bound is satisfactory for small n ($\sim n^2\cdot\lambda_1$) and is essentially given by $\lambda_n = n\ \varphi_n$ with $\varphi_n \sim n\cdot\lambda_1$ which is the first term in our recent new strategy in terms of block's partition [7].
Moreover, we add that the behavior $\lambda_n = n^2\cdot\lambda_1$ is also obtained from our closed set of equations for the Li-Keiper coefficients studied recently. In fact, from [8] the closed set is given by

$$\lambda_n \cong \sum_{k=1}^{n-1} (-1)^{n+k-1} \binom{n}{k} \cdot \lambda_k \tag{6}$$

See Appendix 1 for additional calculations and proofs.

IV. Conclusion

We have presented the analytical as well as the numerical results i.e. upper and lower bounds for the first few Li-Keiper coefficients. To the best of our knowledge these are news or have not been obtained along our lines above.

Additional strategies involving concepts as partitions have also been pursued by us in a recent work [7] and a refinement valid to higher values of n is under analysis and will appear in the near future. The main message here is that the two-body system (2N=2) provides a lower bound for the coefficients involving the Koebe function; an upper bound of the same (given by the present spin model, in n^2- not of interest - for big values of n) is obtained by a limit $2N\rightarrow\infty$ of the system. Moreover, for a $2\cdot N=56$ spin model, we have obtained a truncation of the function ξ, a polynomial, of degree 56 where all zeros in z (z=1-1/s) are on the unit circle (in the variable s =1/(1-z) on the critical line) and where the first 28 Li-Keiper coefficients are very near to the true values λ_n.

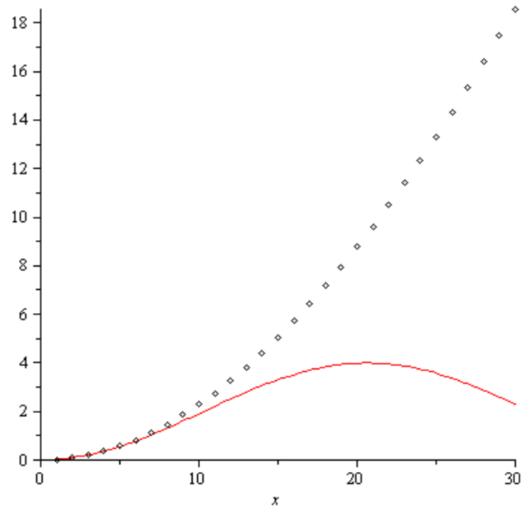

Fig. 2. Riemann Wave background [1,2] (in red) and the first true values of the coefficients λ_n [9](in black).

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Appendix 1

In relation to the numerical values given in the Table 2 we now present more calculations and proof.
A closed set of equations as an approximation to the Li-Keiper coefficients, given by our Eq.(6) is as follows.
Let a binomial transform i.e. Eq.(6) be written as:

$$a_n = \sum_{k=1}^{n-1} (-1)^{n+k-1} \binom{n}{k} \cdot a_k$$

Then, with a_1 and a_2 as initial conditions, we obtain the following solution, sum of arithmetic progressions ∀n:

$$a_n = \frac{n \cdot (n-1)}{2} \cdot a_2 - n \cdot (n-2) \cdot a_1 = n^2 \cdot \left(\frac{a_2}{2} - a_1\right) + n \cdot \left(2 \cdot a_1 - \frac{a_2}{2}\right)$$

Some cases:

1) If $a_2=2\cdot a_1 \rightarrow a_n=n\cdot a_1$, i.e. a linear law given by $\lambda_n=n\cdot\lambda_1$.
2) If $a_2=4\cdot a_1 \rightarrow a_n=n^2\cdot a_1$, i.e. a quadratic law given by $\lambda_n=n^2\cdot\lambda_1$ (the case of the spin system, but only that with a constant two-body interaction=$e^{-2\beta J}$ between two-spins, i.e. J is independent of the distance).
3) If

$$a_n = \frac{n\cdot(n-1)}{2} \cdot a_2 - n \cdot (n-2) \cdot a_1$$

But where a_2 is not related to a_1, we still have a quadratic law for λ_n, given by:

$$\lambda_n = \frac{n \cdot (n-1)}{2} \cdot \lambda_2 - n \cdot (n-2) \cdot \lambda_1 =$$

$$= n^2 \cdot \left(\frac{\lambda_2}{2} - \lambda_1\right) + n \cdot \left(2 \cdot \lambda_1 - \frac{\lambda_2}{2}\right)$$

$\frac{\lambda_2}{2} - \lambda_1 < \lambda_1$, i.e. $\lambda_2 < 4 \cdot \lambda_1$ if λ_2 is the true value: the solution in still quadratic in n, i.e. not interesting for big values of n (if RH is true the dominant term of λ_n is given by $\frac{n}{2} \cdot \ln n$).
Then, we look at an asymptotic solution of Eq.(6) which possibly correctly describes the numerical results for λ_n given in [8], now in the form:

$$a_n = \sum_{k=1}^{n-1} \left(\alpha \cdot k \cdot \ln k + \beta \cdot k + \gamma \cdot \sqrt{n} \cdot \ln k + \delta \cdot \frac{1}{k}\right) (-1)^{n+k-1} \binom{n}{k} = \sum_{k=1}^{n-1} a_k (-1)^{n+k-1} \cdot \binom{n}{k}$$

We then check that as n increases, the solution which we obtain is asymptotically given by:
$a_n \cong \alpha \cdot n \cdot \ln n + \beta \cdot n + \gamma \cdot \sqrt{n} \cdot \ln n$

Then, with α=1/2 and β= -1.13033.. [9, 10] we have [8]:

$$\lambda_n \cong \frac{1}{2} \cdot n \cdot \ln n - 1.13033 \cdot \mathrm{n} + \left(\gamma \cdot \sqrt{n} \cdot \ln n\right) + \delta \cdot (\ln n + 0.57 \ldots)$$

$$\lambda_n = \sum_{k=1}^{n-1} (-1)^{n+k-1} \binom{n}{k} \cdot \left[\frac{1}{2} \cdot k \cdot \ln k - 1.13033 \cdot k \pm \frac{1}{70} \cdot \left(\sqrt{k} \cdot \ln k\right) \pm 0.8 \cdot \frac{1}{k}\right]$$

On the table below, we check our set of closed equations given by Eq.(6), i.e.

$$\lambda_n^* = \sum_{k=1}^{n-1} (-1)^{n+k-1} \binom{n}{k} \cdot \lambda_k^* \qquad (*)$$

After the insertion for λ_k^* the first n-1 λ_k's true values to 12 digits taken from faf448 [9, 10] and compared with the true values, we obtain the table below.

Eq.(*)	relationship	True values
λ_1^*= 0.023095708966	=	0.023095708966
λ_2^*= 0.092345735228	=	0.092345735228
λ_3^*= 0.207750078786	>	0.207638920554
λ_4^*= 0.368864106712	>	0.368790479492
λ_5^*= 0.575541999370	<	0.575542714460
λ_6^*= 0.827565730836	<	0.827566012278
λ_7^*= 1.124460119834	>	1.124460117570
λ_8^*= 1.465755682829	>	1.465755677147
λ_9^*= 1.850916040314	<	1.85091604838
λ_{10}^*= 2.27933937718	>	2.27933936319
λ_{11}^*= 2.750360814863	<	2.75036083822
λ_{12}^*= 3.263255358123	>	3.26325532062