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On the Distribution and Gap Structure of Lee–Yang Zeros for the Ising Model: Periodic and Aperiodic Couplings

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In this work, we present some results on the distribution of Lee–Yang zeros for the ferromagnetic Ising model on the rooted Cayley Tree (Bethe Lattice), assuming free boundary conditions, and in the one-dimensional lattice with periodic boundary conditions. In the case of the Cayley Tree, we derive the conditions that the interactions between spins must obey in order to ensure existence or absence of phase transition at finite temperature ($T \neq 0$). The results are first obtained for periodic interactions along the generations of the lattice. Then, using periodic approximants, we are also able to obtain results for aperiodic sequences generated by substitution rules acting on a finite alphabet. The particular examples of the Fibonacci and the Thue-Morse sequences are discussed. Most of the results are obtained for a Cayley Tree with arbitrary order d. We will be concerned in showing whether or not the zeros become dense in the whole unit circle of the fugacity variable. Regarding the one-dimensional Ising model, we derive a general treatment for the structure of gaps (regions free of Lee–Yang zeros) around the unit circle.

KEY WORDS: Lee–Yang zeros; aperiodic systems; substitution sequences.

1. INTRODUCTION

The ferromagnetic Ising model on a finite lattice L, with pair interactions and under a constant external magnetic field H, is described by the Hamiltonian

$$\mathscr{H}_L = -\sum_{i,j \in L} J_{ij}\sigma_i\sigma_j - \sum_{i \in L} H\sigma_i, \tag{1}$$

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with $J_{ij} \geqslant 0$ and $\sigma_i = \pm 1$. See ref. 1 for historical remarks. It is well known that the partition function of this model is a polynomial of degree $\#L$ (the cardinality of the lattice L) on the fugacity variable $z = e^{-2\beta H}$, β being the inverse temperature. This fact implies the existence of $\#L$ zeros for the partition function as a function of z in the complex plane. A celebrated theorem due to T. D. Lee and C. N. Yang[2, 3] (see also ref. 4 and, for generalisations, ref. 5) states that, for free boundary conditions, the locus of the set of zeros on the complex plane has a simple geometrical description: the zeros are all contained in the unit circle $S^1 = \{z \in \mathbb{C} | |z| = 1\}$.

Lee and Yang's circle theorem has important consequences on what concerns the mechanisms leading to the ferromagnetic phase transition exhibited by the model in certain lattices when the thermodynamic limit $\#L \to \infty$ is taken. From the mathematical side, Lee and Yang's circle theorem attracted much interest due to its deep-lying relation to Number Theory and Analysis, in particular, and more remarkably, to properties of the Riemann zeta function (see ref. 6 for a review and for additional references).

As first observed in refs. 2 and 3, many thermodynamic properties of the Ising model are related to the distribution of the zeros in S^1. There are, however, very few systems for which the relation between the partition function and the fugacity variable is known sufficiently well in order to allow a detailed study of the distribution of zeros when the thermodynamic limit is taken. Among these, are the one-dimensional model and the models defined on the Cayley tree (see below), two systems we will study in this paper.

For such lattices, it has been known for a while that, when the couplings J_{ij} are configured in periodic or aperiodic patterns, the distribution of zeros exhibits an interesting structure of gaps. It has been observed in refs. 7 and 8 that in the one-dimensional case the gaps are apparently classifiable according to Bellissard's gap labelling theorem.[10] Bellissard's theorem was proven in the context of the spectral analysis of one-dimensional Schrödinger operators through the study of K-theoretical properties of certain suitably defined C*-algebras generated by the Hamilton operators. Although no proof of this relation between Bellissard's theorem and the gaps of Lee–Yang zeros is known at the present, this surprising relation points to a possible connection between the Lee–Yang zeros and K-theoretical properties of certain C*-algebras somehow related to the Ising model.[3]

[3] These algebras have not been identified yet, but we conjecture that they are related to the cross product algebras associated to the mappings τ_z of the unit circle S^1, introduced in ref. 11.

In this paper we will not enter into those important but still rather incipient and speculative algebraic questions. Instead, we employ the methods of ref. 11 to analyse properties of the distribution of Lee–Yang singularities of a one-point function for the Ising model on a rooted Cayley tree with periodic and aperiodic configurations of couplings in terms of properties of suitably defined dynamical systems. These results will be described in the next section. In particular, we will present necessary and sufficient conditions on the couplings in order to guarantee that the set of Lee–Yang zeros becomes dense in the whole unit circle when the thermodynamic limit is taken.

The methods employed here do not lead to a detailed analysis of the gap structure of the Lee–Yang zeros on the Cayley tree but, in the somewhat similar case of the one-dimensional model, many general results on the gaps have been found using transfer matrix methods, and will be described in the last sections. We have proved that the regions where the zeros become dense and, hence, the gaps, depend only on the values of the interactions and their frequencies in the chains. Since the open one-dimensional chain and the Cayley tree lead to very similar dynamical systems we believe that analogous results also hold on the Cayley tree. The lack of a transfer matrix formalism for the Cayley tree, however, inhibits the proof of such generalisations.

2. THE CAYLEY TREE. DESCRIPTION OF THE RESULTS

Let C_d denote the rooted Cayley Tree of order d. This lattice has $(d+1)$ bonds attached to each site, except for the root, which has only d bonds. Let us first consider the finite Cayley Tree with M generations.

We say that the root is the generation 0 of the sites. The generation i is the set of sites whose minimal path connecting to the root is composed of i bonds. With this convention the three sites connected to the root in Fig. 1 belong to the first generation, and so forth. Let J_i denote the intensity of the

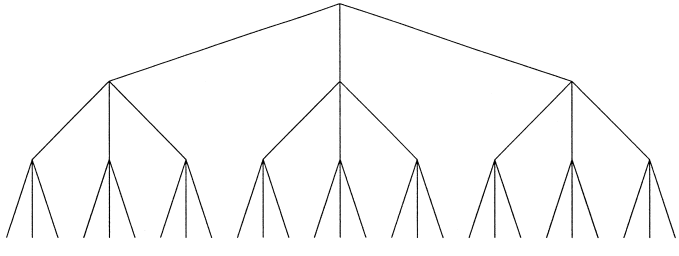


Fig. 1. Rooted Cayley Tree with $d=3$ and $M=3$.

interaction between spins located at sites of the generations i and $i-1$. We will introduce the variables ρ_i defined by $\rho_i = e^{-2\beta J_i}$.

Considering free boundary conditions, the partition function Z_M can be calculated recursively, starting from the last generation and moving towards the root:

$$Z_M = z^{-1/2} Z_0^+ + z^{1/2} Z_0^-, \tag{2}$$

where $Z_j^{\pm}$ are obtained recursively backwards by

$$Z_j^{\sigma} = \left[\sum_{\sigma' = \pm 1} e^{\beta J_j \sigma\sigma'} e^{\beta h \sigma'} Z_{j+1}^{\sigma'} \right]^d$$

with $Z_M^{\pm} = 1$. For the constant case $\rho_i = \rho$, the singularities of the function from which the magnetisation at the origin is derived,

$$\langle \sigma_0 \rangle_M = \frac{1}{Z_M} \sum_{\sigma} \sigma_0 e^{-\beta H(\sigma)} = \frac{1 - z\Delta_0}{1 + z\Delta_0}, \tag{3}$$

have been studied in ref. 11. Above, $\Delta_j = Z_j^- / Z_j^+$. In that work, it has been shown that the problem of locating the Lee–Yang singularities was related to the study of a convenient discrete dynamical system. For $d = 2$ and constant interactions, the dynamical system can be written as

$$\phi_0 = \phi \tag{4}$$

$$\phi_{i+1} = \phi_0 + L(\phi_i), \tag{5}$$

where

$$L(\theta) = 2\theta - 4 \arctan\left(\frac{\rho \sin(\theta)}{1 + \rho \cos(\theta)} \right). \tag{6}$$

In ref. 11, it was observed that the Lee–Yang zeros in the fugacity variable are the values of $z = e^{i\phi}$ such that, starting with $\phi_0 = \phi$, the dynamical system would lead us, after M iterations, to a value ϕ_M satisfying $\cos \phi_M = -1$.

In the following section we wish to generalise these results to the case where the interactions are not constant along the lattice, but vary in a periodic way along the generations. In the next sections we will derive the following quite general result:

Theorem 1. Let C_d denote the rooted Cayley Tree with order d, in the thermodynamic limit. Let the interaction between spins of the genera-

tions $i-1$ and i be J_i for $1 \leqslant i \leqslant p$ and $J_{i+p}=J_i$ for all i. The Lee–Yang zeros are dense in the whole unit circle $|z|=1$ if and only if

$$\Lambda(\rho_1, \rho_2, ..., \rho_p)=d^p \left(\frac{1-\rho_1}{1+\rho_1}\right)\left(\frac{1-\rho_2}{1+\rho_2}\right)\cdots\left(\frac{1-\rho_p}{1+\rho_p}\right) \geqslant 1. \tag{7}$$

If $\Lambda(\rho_1, \rho_2, ..., \rho_p) < 1$, there is at least one gap free of Lee–Yang zeros in the unit circle, around $z=1$.

First, we will derive this result for the case where the periodic Cayley Tree is generated by repetition of the word ab, leading to the sequence of interactions $J_aJ_bJ_aJ_b\cdots$. This is the case of period $p=2$. Then, we will obtain the quite general result for arbitrary order d and period p, where the sequence of interactions is generated by repetition of a general word $\omega=\omega_1\omega_2\cdots\omega_p$ of length p (the length here is defined as the number of letters).

Finally, we will also discuss the case where the interactions along the generations are aperiodic and given by sequences generated by substitution rules on a finite alphabet. The specific examples of the Fibonacci and the Thue-Morse chains are discussed, but we adopt a quite general approach that can be used with any substitutional sequence.

The literature on the zeros of the partition function of the Ising model on hierarchical lattices is very large and a more detailed list of references can be found, for instance, in ref. 7. A common ingredient of many of these works is the identification of the locus of the partition function zeros (in the thermodynamic limit) with the Julia set of some discrete dynamical system, typically interpreted as a renormalization group transformation of some physical parameter. This is the origin of the typical fractal structures exhibited by the distribution of partition function zeros for such lattices.

For the case of the Lee–Yang (fugacity) zeros on the Cayley tree, this can be seen, for instance, in ref. 11 (and other references quoted there), where the discrete dynamical system induced by the mappings τ_z of the unit circle S^1 (introduced in ref. 11) can be interpreted as a renormalization group transformation for the fugacity. As discussed in ref. 11, the Julia set of this discrete dynamical system coincides with the accumulation region of Lee–Yang zeros on the circle when the thermodynamic limit is taken.

For the temperature zeros, also called Fisher zeros, we refer the interested reader to the work of Derrida, de Seze and Itzykson[13] concerning the Ising model on the diamond lattice, where the locus of the partition function zeros is identified with the Julia set of a renormalization group transformation for the variable $e^{-\beta J}$.

3. THE PERIODIC CASE

Let us first consider the Cayley Tree with two different values of the interaction between spins: J_a and J_b. Let $J_i = J_a$ for i odd and $J_i = J_b$ for i even. From the root to the last generation of sites, we have the sequence of interactions $J_a J_b J_a J_b \cdots$. Under these conditions we say that the periodic sequence is generated by the word ab. Defining the variables $\rho_a = e^{-2\beta J_a}$ and $\rho_b = e^{-2\beta J_b}$ we have two different functions

$$L_a(\theta) = 2\theta - 4 \arctan\left(\frac{\rho_a \sin(\theta)}{1+\rho_a \cos(\theta)}\right),$$

$$L_b(\theta) = 2\theta - 4 \arctan\left(\frac{\rho_b \sin(\theta)}{1+\rho_b \cos(\theta)}\right).$$

The dynamical system to be discussed can be written as

$$\begin{aligned} &\phi_0 = \phi \\ &\phi_1 = \phi_0 + L_a(\phi_0) \\ &\phi_2 = \phi_0 + L_b(\phi_1) = \phi_0 + L_b(\phi_0 + L_a(\phi_0)) \\ &\vdots \end{aligned} \tag{8}$$

As in ref. 11, the Lee–Yang zeros are located at the angles ϕ such that $\phi_0 = \phi$ implies $\cos \phi_M = -1$. We are interested in the properties of the system in the thermodynamic limit $M \to \infty$. In order to keep the periodic property, we will increase the number of generations by two in each step. It is therefore natural to define a new dynamical system

$$\begin{aligned} &\phi_0 = \phi \\ &\phi_1 = \phi_0 + L_b(\phi_0 + L_a(\phi_0)) \\ &\vdots \\ &\phi_{i+1} = \phi_0 + L_b(\phi_0 + L_a(\phi_i)) = \phi_0 + U_{\phi_0}(\phi_i). \end{aligned} \tag{9}$$

Above, we have defined $U_{\phi_0}(\phi) = L_b(\phi_0 + L_a(\phi))$ to keep the notation as simple as possible. Each iteration of the new dynamical system is equivalent to two iterations of the previous one. Using the relation

$$L_j'(x) = 2\left(\frac{1-\rho_j^2}{1+2\rho_j \cos x + \rho_j^2}\right) \geqslant 2\left(\frac{1-\rho_j^2}{(1+\rho_j)^2}\right) = 2\frac{1-\rho_j}{1+\rho_j}, \tag{10}$$

we have

$$U'_{\phi_0}(x) = L'_b(\phi_0 + L_a(x))\, L'_a(x) \geqslant 4\,\frac{1-\rho_a}{1+\rho_a}\,\frac{1-\rho_b}{1+\rho_b} = \Lambda(\rho_a, \rho_b). \tag{11}$$

Let us first obtain the behaviour of the distribution of zeros when the following inequality holds:

$$\Lambda(\rho_a, \rho_b) \geqslant 1, \tag{12}$$

what is equivalent to $4(1-\rho_a)(1-\rho_b) \geqslant 1+\rho_a+\rho_b+\rho_a\rho_b$. In terms of ρ_a we have the inequality

$$\rho_a \leqslant \frac{3-5\rho_b}{5-3\rho_b}. \tag{13}$$

Figure 2 presents the curve $\Lambda(\rho_a, \rho_b)=1$ in the space defined by the variables ρ_a and ρ_b. The region characterised by $\Lambda(\rho_a, \rho_b) \geqslant 1$ is bounded by the curve and the two axis.

As a result of the Lee–Yang Circle theorem, the partition function on the Cayley Tree with n generations has $2^{2n}-1$ zeros in the unit circle of the fugacity variable. Moreover, by the same arguments of ref. 11, the zeros are all distinct. In the upper half plane, we can label the zeros $z(n, l) = e^{i\phi(n,l)}$, $1 \leqslant l \leqslant 2^n$, in increasing order of angle, using the increasingly ordered set $\{\phi(n, l) \in [0, \pi], 1 \leqslant l \leqslant 2^n\}$. Since the zeros are all distinct, we can ensure that $\phi(n, l') > \phi(n, l)$ if $l' > l$.

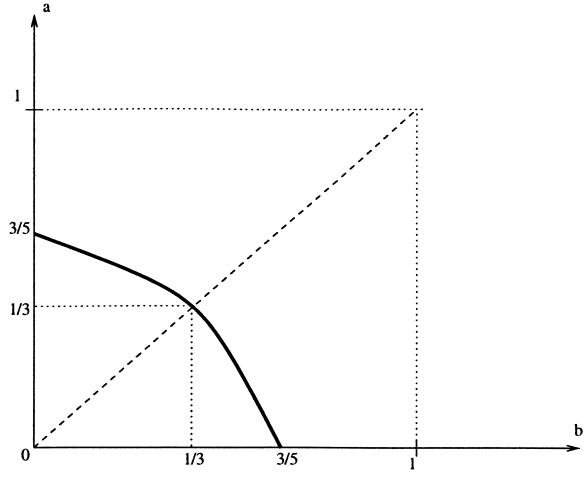


Fig. 2. Curve $\Lambda(\rho_a, \rho_b)=1$ in the space (ρ_a, ρ_b).

The first question that rises is what happens when the thermodynamic limit is taken to the distance between two consecutive zeros, $\phi(n, l+1)$ and $\phi(n, l)$. Defining $\phi_i(n, l)$ as the i-th iteration started form $\phi(n, l)$, we have for $0 \leqslant i \leqslant n-1$

$$\phi_{i+1}(n, l+1) - \phi_{i+1}(n, l) = \phi(n, l+1) - \phi(n, l) + U_{\phi_0(n, l+1)}(\phi_i(n, l+1)) - U_{\phi_0(n, l)}(\phi_i(n, l)). \tag{14}$$

Since

$$\frac{\partial U_{\phi_0}}{\partial \phi_0} = L_b'(\phi_0 + L_a(x)) \geqslant 0, \tag{15}$$

we have,

$$U_{\phi_0(n, l+1)}(\phi_i(n, l+1)) > U_{\phi_0(n, l)}(\phi_i(n, l+1)). \tag{16}$$

Therefore, the distance between the $(i+1)$-th iteration of two successive zeros is bounded by

$$\begin{aligned}
&\phi_{i+1}(n, l+1) - \phi_{i+1}(n, l) \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + U_{\phi_0(n, l+1)}(\phi_i(n, l+1)) - U_{\phi_0(n, l)}(\phi_i(n, l)) \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + \int_{\phi_i(n, l)}^{\phi_i(n, l+1)} U'_{\phi_0(n, l)}(x)\, dx \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + \Lambda(\phi_i(n, l+1) - \phi_i(n, l)) \\
&\quad \geqslant \left(\sum_{k=0}^{i} \Lambda(\rho_a, \rho_b)^k \right) (\phi(n, l+1) - \phi(n, l)).
\end{aligned} \tag{17}$$

Taking into account the relation $\phi_n(n, l+1) - \phi_n(n, l) = 2\pi$, we can take $i = n-1$ to derive from (17)

$$\phi(n, l+1) - \phi(n, l) \leqslant 2\pi \left(\sum_{k=1}^{n-1} [\Lambda(\rho_a, \rho_b)]^k \right)^{-1}. \tag{18}$$

Hence, if $\Lambda(\rho_a, \rho_b) \geqslant 1$, the sum diverges for $n \to \infty$, resulting in

$$\lim_{n \to \infty} (\phi(n, l+1) - \phi(n, l)) = 0. \tag{19}$$

To complete the proof that the Lee–Yang zeros are dense in the unit circle of the fugacity variable, we need to show that $\phi(n, 1)$ goes to zero as the thermodynamic limit is taken. In fact,

$$\begin{aligned}\phi_{i+1}(n, 1) &= \phi(n, 1) + U_{\phi(n,1)}(\phi_i(n, 1)) \geqslant \phi(n, 1) + U_0(\phi_i(n, 1)) \\ &\geqslant \phi(n, 1) + \int_0^{\phi_i(n,1)} U_0'(x)\, dx \geqslant \phi(n, 1) + \Lambda(\rho_a, \rho_b)\, \phi_i \\ &\geqslant \phi(n, 1) \left(\sum_{k=0}^{i} [\Lambda(\rho_a, \rho_b)]^k \right). \end{aligned} \tag{20}$$

Setting $i = n-1$, the previous inequality can be combined with $\phi_n(n, 1) = \pi$ to derive

$$\phi(n, 1) \leqslant \pi \left(\sum_{k=0}^{n-1} [\Lambda(\rho_a, \rho_b)]^k \right)^{-1}. \tag{21}$$

Therefore, in the thermodynamic limit, the right hand side goes to zero, and we obtain

$$\lim_{n \to \infty} \phi(n, 1) = 0. \tag{22}$$

Since the Lee–Yang zeros are dense around $z = 1$, the magnetisation at the origin cannot be analytically continued from $H < 0$ to $H > 0$ or, in terms of the fugacity, from $z < 1$ to $z > 1$. This lack of analyticity is regarded as a phase transition.

We shall next establish that in the complementary region $\Lambda(\rho_a, \rho_b) < 1$ the closure of the set of Lee–Yang zeros is a proper subset of the unit circle. More precisely, we shall prove that there is at least one gap free of zeros, around $\phi = 0$. This gap prevents the existence of phase transition at finite temperature, since there is no lack of analyticity of the thermodynamic functions for the whole interval $0 \leqslant z < \infty$.

If $\Lambda(\rho_a, \rho_b) < 1$, it is possible to find k_1 such that, for all $\phi_0 < k_1$ we have $U'_{\phi_0}(0) < 1$. To obtain the value of k_1, all we have to do is solve the inequality

$$U'_{\phi_0}(0) = 4 \left(\frac{1 - \rho_b^2}{1 + 2\rho_b \cos \phi_0 + \rho_b^2} \right) \left(\frac{1 - \rho_a}{1 + \rho_a} \right) = \Lambda(\rho_a, \rho_b) \frac{(1 + \rho_b)^2}{1 + 2\rho_b \cos \phi_0 + \rho_b^2} < 1. \tag{23}$$

It is straightforward to show that

$$\cos k_1 = \frac{\Lambda(\rho_a, \rho_b)(1 + \rho_b)^2 - 1 - \rho_b^2}{2\rho_b}, \tag{24}$$

when the right hand side is greater than one and $k_1 = \pi$ otherwise. It is crucial to assume that $\Lambda(\rho_a, \rho_b) < 1$; otherwise, the right hand side would be a number greater than one, and there would be no possible k_1.

Moreover, it is not difficult to see that the second derivative of U_{ϕ_0} is positive for sufficiently small angles. Therefore, one can find $k_2 < k_1$ small enough such that equation

$$\phi_0 + U_{\phi_0}(\phi) = \phi \tag{25}$$

has at least one solution in the interval $[0, \pi)$. After rather long calculations, one could obtain a mathematically rigorous proof of the last statement. Instead of taking this approach, we will use a graphical method which provides a natural way to understand what happens to the dynamical system. Figure 3 presents the graph of the functions $g(\phi) = \phi_0 + U_{\phi_0}(\phi)$ and $f(\phi) = \phi$. The dashed lines indicate the evolution of the dynamical system starting from $\phi_0 < k_2$. The system converges to a value $\omega(\phi_0)$ that is the smallest among the solutions of (25).

Looking in more detail at the graph, we see that k_2 is given by the intersection of the y-axis with the curve $g(\phi)$ that is tangent to $f(\phi)$. To obtain this value, we have to solve the following equations:

$$k_2 + U_{k_2}(\omega) = \omega \tag{26}$$

$$U'_{k_2}(\omega) = L'_b(k_2 + L_a(\omega))\, L'_a(\omega) = 1 \tag{27}$$

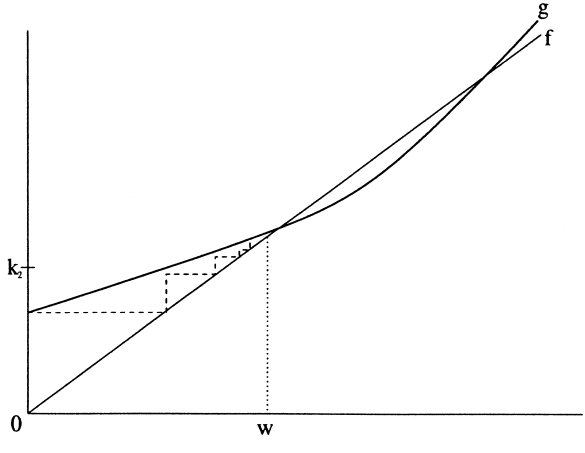


Fig. 3. Functions $g(\phi) = \phi_0 + U_{\phi_0}(\phi)$ and $f(\phi) = \phi$.

Summarising, taking $\phi_0 < \min\{k_2, \pi\}$ as the starting point, the dynamical system converges to a value that is smaller than π, in such a way that $\cos \phi_M > -1$ and $z = e^{i\phi_0}$ cannot be a Lee–Yang zero. Therefore, the whole interval $[-k_2, k_2]$ is free of zeros of the partition function and there is a gap around $z = 1$.

We have concluded the proof of the following theorem:

Theorem 2. Let C_2 denote the rooted Cayley Tree with order $d = 2$, in the thermodynamic limit. Let the interaction between spins of the generations i and $i+1$ be J_a for i even and J_b for i odd. The Lee–Yang zeros are dense in the whole unit circle $|z| = 1$ if and only if

$$\Lambda(\rho_a, \rho_b) = 4 \frac{1-\rho_a}{1+\rho_a} \frac{1-\rho_b}{1+\rho_b} \geqslant 1. \tag{28}$$

This condition is equivalent to

$$\rho_a \leqslant \frac{3-5\rho_b}{5-3\rho_b}. \tag{29}$$

If $\Lambda(\rho_a, \rho_b) < 1$, there is at least one gap free of Lee–Yang zeros in the unit circle, around $z = 1$.

It is interesting to note that, provided J_a is sufficiently small, the zeros are not dense in the unit circle, regardless of the value of J_b. Let J_a^* denote the suppremum of the values of J_a that satisfy this property. In the conditions of the previous theorem, we have $\rho_a^* = 3/5$, or

$$e^{-2\beta J_a^*} = 3/5 \to J_a^* = \frac{kT}{2} \ln \frac{5}{3}. \tag{30}$$

For $J_a < J_a^*$ the phase transition no longer occurs, regardless of how large J_b can be.

4. GENERIC PERIOD *p* AND ORDER *d*

For arbitrary period p, the Liapunov exponent of the dynamical system is related to the logarithm of the function

$$\Lambda(\rho_1, \ldots, \rho_p) = 2^p \prod_{i=1}^{p} \left(\frac{1-\rho_i}{1+\rho_i} \right). \tag{31}$$

The hypersurface $\Lambda(\rho_1, ..., \rho_p)=1$ is the boundary of the region of parameters for which the Lee–Yang zeros become dense when the thermodynamic limit is taken.

We can generalise even further and consider the Tree with order d. In this case, the recursive relation for the partition function should be written as

$$Z_j^{\sigma}=\left[\sum_{\sigma'=\pm 1} e^{\beta J_j \sigma\sigma'} e^{\beta h\sigma'} Z_{j+1}^{\sigma'}\right]^d.$$

This relation will result in a new function:

$$L_j(\theta)=d\left(\theta-2\arctan\left(\frac{\rho_j \sin(\theta)}{1+\rho_j \cos(\theta)}\right)\right). \tag{32}$$

Therefore, the properties of the system will be closely related to the behaviour of the function

$$\Lambda^{(d)}(\rho_1, ..., \rho_p)=d^p \prod_{i=1}^{p}\left(\frac{1-\rho_i}{1+\rho_i}\right). \tag{33}$$

In the case of period $p=2$, the region $\Lambda(\rho_1, \rho_2) \geqslant 1$ will be

$$\rho_1 \leqslant \frac{(d^2-1)-(d^2+1)\,\rho_2}{(d^2+1)-(d^2-1)\,\rho_2} \tag{34}$$

and the limit interaction for the possibility of having a phase transition is obtained by setting $\rho_b=0$ in the right hand side:

$$\rho_1^*=\frac{d^2-1}{d^2+1} \rightarrow J_a^*=\frac{kT}{2}\ln\frac{d^2+1}{d^2-1}. \tag{35}$$

For arbitrary period p, each interaction has a limit value given implicitly by $\Lambda(\rho_1, 0, 0, ..., 0)=1$

$$d^p\left(\frac{1-\rho_1^*}{1+\rho_1^*}\right)=1 \tag{36}$$

or

$$\rho_1^*=\frac{d^p-1}{d^p+1} \rightarrow J_1^*=\frac{kT}{2}\ln\left[\frac{d^p+1}{d^p-1}\right]. \tag{37}$$

The approach adopted in the previous section is recommended when the number of different interactions is exactly equal to the period. Should any constraint among the interactions occur, we should try a slightly different method, which we will briefly describe.

Let us first consider the chain with period $p=3$ generated by repetition of the word *abb*. In this case, the period is greater than the number of distinct interactions, and the previous method is not recommended. However, it can be slightly modified to provide the solution of the problem.

Starting with the periodic chain generated by the word *abc*, our previous method indicates that the region in the space of interactions which corresponds to a dense set of zeros in the whole unit circle is limited by the surface

$$\Gamma(\rho_a, \rho_b, \rho_c)=8\left(\frac{1-\rho_a}{1+\rho_a}\right)\left(\frac{1-\rho_b}{1+\rho_b}\right)\left(\frac{1-\rho_c}{1+\rho_c}\right)=1. \tag{38}$$

This is a convex surface, which contains the point (1/3, 1/3, 1/3), and crosses the axis at the values

$$\rho=\frac{2^p-1}{2^p+1}=\frac{7}{9}. \tag{39}$$

The case of the word *abb* corresponds to $\rho_b=\rho_c$. Therefore, we can take the intersection of the curve with the plane $\rho_b=\rho_c$, and project it into the plane $\rho_c=0$.

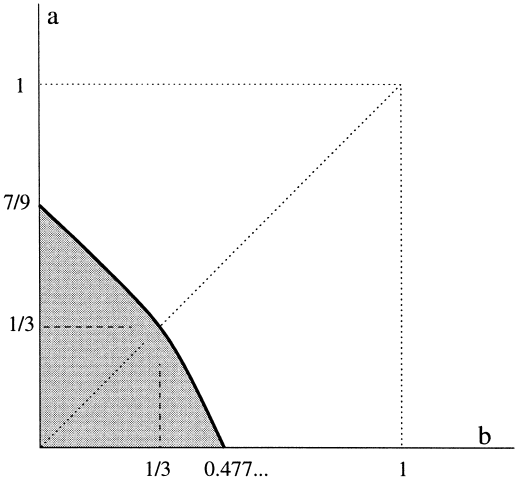


Fig. 4. Solution for the sequence *abbabbabb*....

We already know that the curve crosses the a-axis at $\rho_a = 7/9$. In order to obtain the value where it crosses the b-axis (that must be a number between 1/3 and 7/9), one should take the exact expression

$$\Gamma(\rho_a, \rho_b, \rho_c) = 8\left(\frac{1-\rho_a}{1+\rho_a}\right)\left(\frac{1-\rho_b}{1+\rho_b}\right)^2 = 1 \tag{40}$$

and set $\rho_a = 0$. We have

$$\rho_b = \frac{\sqrt{8}-1}{\sqrt{8}+1} = 0.4776\ldots. \tag{41}$$

When comparing the region bounded by the curve with the one from the previous example (ab), we notice that the region which corresponds to $\rho_a < 1/3$ and $\rho_b > 1/3$ increases, as the region bounded by the curve and the constraints $\rho_a > 1/3$ and $\rho_b < 1/3$ decreases. We should not be surprised with this fact, since it indicates the increase in importance of the interaction J_b in the determination of the behaviour of the system, provided that it occurs twice as frequently as J_a in the sequence of couplings.

In fact, in the case of arbitrary period, the curve depends only on the relative frequency of the interactions in the sequence. Our analysis will be now restricted to the case of two different interactions. For instance, taking the sequence generated by repetition of the word *baabab*, the condition for existence of phase transitions is:

$$2^6\left(\frac{1-\rho_a}{1+\rho_a}\right)^3\left(\frac{1-\rho_b}{1+\rho_b}\right)^3 \geqslant 1. \tag{42}$$

Taking the square root, we reproduce exactly the condition obtained in the case of period $p = 2$. Analogously, the results obtained for the chain *abbabbabb*... can be applied in the study of all chains where the proportion of letters a and b is 1 : 2, as in *baabbbbaabbb*... and *babbbababbba*....

For the periodic chain, where the generating word has n_a letters a and n_b letters b with $n_a + n_b = p$, $n_a/p = f_a$ and $n_b/p = n_b$, we have the curve

$$2^p\left(\frac{1-\rho_a}{1+\rho_a}\right)^{n_a}\left(\frac{1-\rho_b}{1+\rho_b}\right)^{n_b} = 1. \tag{43}$$

Taking the p-th root,

$$2\left(\frac{1-\rho_a}{1+\rho_a}\right)^{f_a}\left(\frac{1-\rho_b}{1+\rho_b}\right)^{f_b} = 1. \tag{44}$$

Therefore, we have proved that when the values of the interactions are fixed, the existence or absence of phase transition depends only on the frequencies of each of the letters, regardless of the length and the particular sequence of letters in the generating word.

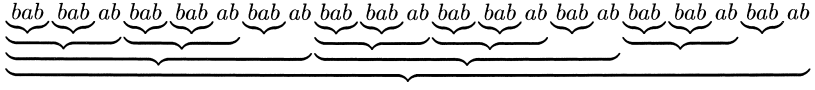
5. THE APERIODIC CASE

We will first consider the Fibonacci chain as a model for treating aperiodic chains. Consider the space $\{a, b\}^{\mathbb{N}}$ of all semi-infinite sequences of words generated by the letters a and b. The *Fibonacci chain* is the fixed point in $\{a, b\}^{\mathbb{N}}$ by the substitution sequence ρ (see the appendix), defined on the alphabet $\{a, b\}$ by

$$\rho(a) = b, \qquad \rho(b) = ba.$$

Its first elements are *babbababbabbababbabab...,* etc.

Although not periodic, the Fibonacci chain contains infinite units with arbitrarily large length repeated in a quasi-periodic way along the chain:



As in the case of almost-periodic functions, which can be approximated by periodic ones, the Fibonacci chain can be approximated, in an intuitive sense that can be made precise, by periodic sequences. We exploit this idea and consider periodic approximants with increasingly large periods for the partition functions defined by the Fibonacci chain. The results we derived in our analysis of periodic sequences are independent of the periods, but depend rather on the frequencies of the letters a and b on the chain. Therefore, that results can be extrapolated to systems defined by aperiodic sequences as well, provided the aperiodic sequences have periodic approximants, as in the Fibonacci case. See refs. 7 and 8 and other references therein.

We will, hence, consider the situation where the sequence of interactions along the generations of the Bethe lattice is given by the Fibonacci chain. Therefore, the interaction between the root and the nearest neighbours sites is J_b, followed by J_a (second generation), J_b, J_b, J_a, etc. We shall only be concerned with the case $d = 2$. Although the sequence of interactions is not periodic, the formalism developed in the last sections can

be used to provide a sufficient but not optimal condition for the existence of phase transition. The dynamical system to be considered is

$$\begin{aligned}
\phi_0 &= \phi \\
\phi_1 &= \phi_0 + L_b(\phi_0) \\
\phi_2 &= \phi_0 + L_a(\phi_1) = \phi_0 + L_a(\phi_0 + L_b(\phi_0)) \\
\phi_3 &= \phi_0 + L_b(\phi_2) \\
\phi_4 &= \phi_0 + L_b(\phi_3). \\
&\vdots
\end{aligned} \tag{45}$$

A brief description of the main results for aperiodic sequences generated by substitution rules is presented in the appendix. The most interested reader can find the complete theory in ref. 12.

In analogy with the periodic case, we will introduce a new dynamical system with ϕ_i restricted to the even values of i. This is equivalent to take two interactions at each step.

To simplify the notation, we define

$$U_{\phi_0}^{(ba)}(\phi) = L_b(\phi_0 + L_a(\phi)) \tag{46}$$

and the analogous functions $U_{\phi_0}^{(bb)}$ and $U_{\phi_0}^{(aa)}$. In the periodic case, we were mainly concerned with the values the case where U'_{ϕ_0} was always greater than one (for $p=2$, this is equivalent to the condition $\Lambda(\rho_a, \rho_b) \geqslant 1$). While dealing with aperiodic chains, this condition will also be sufficient to ensure that the zeros are dense in the unit circle. However, for the Fibonacci sequence, we have three conditions to be satisfied, $\Lambda(\rho_a, \rho_b) \geqslant 1$, $\Lambda(\rho_b, \rho_b) \geqslant 1$ and $\Lambda(\rho_b, \rho_a) \geqslant 1$, where the first and the third one are the equivalent.

Each condition corresponds to one of the combinations $U_{\phi_0}^{(ab)}$, $U_{\phi_0}^{(bb)}$ and $U_{\phi_0}^{(ab)}$. This is a consequence of the occurrence of the two-letter words *ab*, *ba* and *bb* with non-vanishing frequency, and *aa* with zero frequency. This fact, whose proof is deferred to the appendix, can be verified directly from the substitution rule, but the idea can be used in more complicated sequences, even if the alphabet is composed of more than two letters.

Let us suppose for a moment that the two inequalities $\Lambda(\rho_a, \rho_b) = \Lambda(\rho_b, \rho_a) \geqslant 1$ and $\Lambda(\rho_b, \rho_b) \geqslant 1$ hold. The dynamical system for the i-th step can be written as

$$\phi_i = \phi_0 + U_{\phi_0}^{(p_i)}(\phi_{i-1}), \tag{47}$$

where $P_i \in \{ab, ba, bb\}$. Therefore, one can define $\Lambda = \min\{\Lambda(\rho_a, \rho_b), \Lambda(\rho_b, \rho_b)\}$ in order to derive

$$\begin{aligned}
&\phi_{i+1}(n, l+1) - \phi_{i+1}(n, l) \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + U^{(P_{i+1})}_{\phi_0(n, l+1)}(\phi_i(n, l+1)) - U^{(P_{i+1})}_{\phi_0(n, l)}(\phi_i(n, l)) \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + \int_{\phi_i(n, l)}^{\phi_i(n, l+1)} U^{(P_{i+1})'}_{\phi_0}(x)\, dx \\
&\quad \geqslant \phi(n, l+1) - \phi(n, l) + \Lambda(\phi_i(n, l+1) - \phi_i(n, l)) \\
&\quad \geqslant \left(\sum_{k=0}^{i} \Lambda^k \right) (\phi(n, l+1) - \phi(n, l)).
\end{aligned} \tag{48}$$

We are, hence, able now to obtain an upper bound for the distance between two consecutive zeros:

$$\phi(n, l+1) - \phi(n, l) \leqslant 2\pi \left(\sum_{k=1}^{n-1} \Lambda^k \right)^{-1}. \tag{49}$$

When $\Lambda \geqslant 1$, the sum in the right hand side diverges when $n \to \infty$, and the distance goes to zero:

$$\lim_{n \to \infty} (\phi(n, l+1) - \phi(n, l)) = 0. \tag{50}$$

By now, we were able to prove that the Lee–Yang zeros turn out to be dense in a connected subset of the circle. We shall now obtain an upper bound for the first Lee–Yang zero, which is given by

$$\phi(n, 1) \leqslant \pi \left(\sum_{k=0}^{n-1} \Lambda^k \right)^{-1}. \tag{51}$$

In the infinite lattice limit we have again $\lim_{n \to \infty} \phi(n, 1) = 0$, and we have established that the zeros are dense in the unit circle, provided $\Lambda \geqslant 1$.

Figure 5 illustrates the region $\Lambda \geqslant 1$ in the interaction space (ρ_a, ρ_b). One should be careful to notice that we have no information on what happens in the region outside the curve, defined by $\Lambda < 1$. In fact, it will be shown that the region $\Lambda \geqslant 1$ is not the optimal region where the zeros become dense in the unit circle.

In order to obtain the optimal region, we will employ the ideas developed in the last section. More precisely, we have derived that the

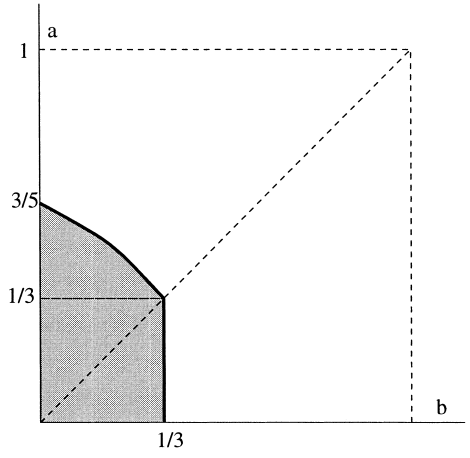


Fig. 5. First approximation for the Fibonacci sequence.

region where the zeros become dense had the curve (44) as its boundary, where the interactions between the generations has only two values J_a and J_b, which is the case of the Fibonacci chain. In other words, it is valid whenever the sequence is based on the alphabet $\{a, b\}$.

In the appendix, it will be shown that the relative frequency of each of the letters in the final chain is given by the normalised eigenvector of the substitution matrix

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \tag{52}$$

that corresponds to its maximal eigenvalue, whose existence is ensured by the Perron–Frobenius Theorem.[4] Thus, we need to obtain the maximal solution λ^+ of the characteristic equation $\det(\lambda I - M) = \lambda^2 - \lambda - 1 = 0$. We have $\lambda^+ = \frac{1+\sqrt{5}}{2}$. The corresponding eigenvector is $v^{(1)} = \binom{f_a}{f_b}$, with

$$f_a = \frac{1}{1+\lambda^+} = 0.3819\ldots,$$

$$f_b = \frac{\lambda^+}{1+\lambda^+} = 0.6180\ldots.$$

$v^{(1)}$ is normalised in such a way that $f_a + f_b = 1$.

[4] Notice that M^2 and higher powers of M have strictly positive entries and, hence, the Perron–Frobenius theorem applies.

The curve (44) crosses the ρ_a-axis in

$$\rho_a = \frac{2^{1/f_a} - 1}{2^{1/f_a} + 1} = 0.7198... > 3/5 \tag{53}$$

and the ρ_b-axis in

$$\rho_a = \frac{2^{1/f_a} - 1}{2^{1/f_a} + 1} = 0.5085... < 3/5. \tag{54}$$

It is clear that this result is an extension of the previous one, since the latter curve lies completely outside the former region. In the region outside the curve (44), there is a gap around $z = 1$, which prevents the existence of phase transition at finite temperature.

This idea can also be used in the case of the Thue-Morse sequence, generated by the following substitution rule:

$$\rho(a) = ab, \qquad \rho(b) = ba, \tag{55}$$

which leads to the chain

$$b \to ba \to baab \to baababba \to baababbaabbabaab \cdots. \tag{56}$$

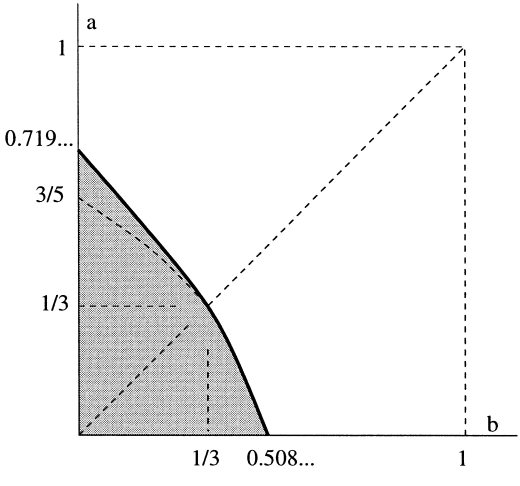


Fig. 6. Optimal region for the Fibonacci sequence.

In this case, the maximal normalised eigenvector which corresponds to the maximal eigenvalue is $v^{(1)}=\binom{1/2}{1/2}$. This is equivalent to say that the two letters, a and b, have the same frequency of occurrence. Therefore, condition for the existence or absence of phase transition is the same as in the case of period $p=2$.

6. THE ONE-DIMENSIONAL MODEL AND THE TRANSFER MATRIX FORMALISM

We shall now discuss the one-dimensional ferromagnetic Ising model with nearest neighbour interactions in an external magnetic field. Assuming periodic boundary conditions, the Hamiltonian for the chain with N sites can be written as

$$\mathscr{H}(\sigma)=-\sum_{i=1}^{N} J_i\sigma_i\sigma_{i+1}-\sum_{i=1}^{N} H\sigma_j,$$

where $\sigma_{N+1}=\sigma_1$. Let $J_j \geqslant 0$ denote the interaction between the j-th and the $(j+1)$-th sites and H is the strength of the external magnetic field.

The partition function of the system can be conveniently written in terms of transfer matrices as

$$Z_N=\mathrm{Tr}(T_1T_2\cdots T_N),$$

where

$$T_j=\begin{pmatrix} z^{1/2}e^{\beta J_j} & e^{-\beta J_j} \\ e^{-\beta J_j} & z^{-1/2}e^{\beta J_j}\end{pmatrix}, \tag{57}$$

where, for convenience, we the fugacity variable now as $z=e^{2\beta H}$.

Since we shall only be concerned with periodic chains, we will assume that the relation $J_{i+p}=J_i$ is valid for all i and for some p which defines the period of the chain. Therefore, the partition function for the chain of length $N=n\cdot p$ is $Z_N=\mathrm{Tr}(T^{(p)})^n$, where $T^{(p)}=T_1T_2\cdots T_p$. As we shall see later, the determinant of $T^{(P)}$ is non-vanishing whenever $\beta^{-1}=T\neq 0$, in such a way that one can define the complex variable ϕ,[7] with real part in $[0,\pi]$, by

$$\cos(\phi)=\frac{\mathrm{Tr}(T^{(p)})}{2\sqrt{\det(T^{(p)})}}. \tag{58}$$

The importance of this variable lies in the fact that the Lee–Yang zeros are uniformly distributed in ϕ, when the thermodynamic limit is taken. This is a consequence of the following equality,[7]

$$Z_n = 2(\det T^{(p)})^{n/2} \cos(n\phi),$$

which can be verified by induction in n. Therefore, the Lee–Yang zeros correspond precisely to the zeros of $\cos(n\phi)$, which are given by the real numbers $\phi = (k-1/2)\,\pi/n$, $k=1, 2, ..., n$. In the limit $N \to \infty$, the distribution of zeros becomes uniform in $[0, \pi]$, in the variable ϕ.

Our purpose in the following section is to derive the general equation (58) in terms of the interactions J_i and the magnetic field H. This general expression is useful in obtaining the structure of gaps (connected regions free of Lee–Yang zeros) that appear in the unit circle of the fugacity variable z. We were able to prove a general proposition (Proposition 1, below), whose most important consequence is the following theorem, which connects the angular variables ϕ and θ, the later being the argument of the fugacity variable z on the complex unit circle. This theorem will be the starting point of our analysis of the gap structure of the Lee–Yang zeros.

Theorem 3. Consider a one-dimensional and periodic lattice, with period p. Let θ be the angle for the unit circle of the fugacity variable: $z = e^{i\theta}$. Let $\tau_i = \exp(2\beta J_i)$ and let also Λ^{p+} denote the set

$$\Lambda^{p+} = \left\{ \{s_i\}_{i=1}^{p},\ s_i = \pm 1,\ \prod_{i=1}^{p} s_i = 1 \right\}. \tag{59}$$

Then, relation (58) can be written as

$$\cos(\phi) = \frac{\displaystyle\sum_{\{s_i\} \in \Lambda^{p+}} \left(\prod_{i=1}^{p} \tau_i^{(s_i - 1)} \right)^{1/2} \cos\left[\frac{\theta}{2} \sum_{i=1}^{p} \prod_{j=1}^{i} s_j \right]}{\left[\displaystyle\prod_{i=1}^{p} (1 - \tau_i^{-2}) \right]^{1/2}}. \tag{60}$$

One can easily see that $\cos\phi$ is a polynomial of order p in $\cos(\theta/2)$. We shall see that the order of the polynomial is related to the maximum number of gaps that can appear in the unit circle.

7. GENERAL RESULTS

In terms of θ and of τ_i, the transfer matrices in the unit circle can be written as

$$T_i = \begin{pmatrix} \tau_i^{1/2} e^{i\theta/2} & \tau_i^{-1/2} \\ \tau_i^{-1/2} & \tau_i^{1/2} e^{-i\theta/2} \end{pmatrix}. \tag{61}$$

We notice that the entries T_{ab}, $a, b = 1, 2$, of these complex matrices have the following properties: $T_{11} = \overline{T_{22}}$ and $T_{12} = \overline{T_{21}}$. It is also interesting to notice that the subspace of 2×2-matrices for which these properties hold is closed under multiplication. Indeed, let B and C be two such matrices. If $A = BC$, then

$$A_{22} = \sum_i B_{2i} C_{i2} = B_{22} C_{22} + B_{21} C_{12} = \overline{B_{11} C_{11}} + \overline{B_{12} C_{21}} = \sum_i \overline{B_{1i} C_{i1}} = \overline{A_{11}}$$

$$A_{21} = \sum_i B_{2i} C_{i1} = B_{21} C_{11} + B_{22} C_{21} = \overline{B_{12} C_{22}} + \overline{B_{11} C_{12}} = \sum_i \overline{B_{1i} C_{i2}} = \overline{A_{12}}.$$

This fact will simplify our calculations.

We wish to obtain a general expression for the trace of $T^{(p)}$. By the discussion above, we will only be concerned with the elements $T_{11}^{(p)}$ and $T_{12}^{(p)}$, since $T_{22}^{(p)}$ and $T_{21}^{(p)}$ can be obtained by complex conjugation.

Since $T^{(p)}$ is the product of p 2×2-matrices with non-vanishing matrix elements, $T_{11}^{(p)}$ is the sum of $2^{(p-1)}$ terms involving products of the matrix elements of T_j for $j = 1, \ldots, p$. From (61), each of these terms is composed by a factor like $\tau_1^{\pm 1/2} \tau_2^{\pm 1/2} \cdots \tau_p^{\pm 1/2}$ times the exponential of an integer multiple of $i\theta/2$. In $T_{11}^{(p)}$, we will find the terms with an even number of negative exponents $\tau_i^{-1/2}$, while $T_{12}^{(p)}$ will be composed by the terms with an odd number of factors $\tau_i^{-1/2}$. Moreover, each positive factor $\tau_i^{1/2}$ contributes with $\theta/2$ to the argument of the exponential when it is preceded by an even number of factors $\tau_j^{-1/2}$, $j < i$, and contributes with $-\theta/2$ when it is preceded by an odd number of such terms. The negative factors do not add any change to the argument of the exponential.

Let us express these results more precisely. Let Λ^{p+} be defined by (59). Analogously, define

$$\Lambda^{p-} = \left\{ \{s_i\}_{i=1}^p, s_i = \pm 1, \prod_{i=1}^p s_i = -1 \right\}.$$

By the discussion above, we should expect to have

$$T_{11}^{(p)} = \sum_{\{s_i\} \in \Lambda^{p+}} \left(\prod_{i=1}^p \tau_i^{s_i} \right)^{1/2} \exp\left[\frac{i\theta}{2} \left(\sum_{i=1}^p \frac{(s_i + 1)}{2} \prod_{j=1}^{i-1} s_j \right) \right],$$

$$T_{12}^{(p)} = \sum_{\{s_i\} \in \Lambda^{p-}} \left(\prod_{i=1}^p \tau_i^{s_i} \right)^{1/2} \exp\left[\frac{i\theta}{2} \left(\sum_{i=1}^p \frac{(s_i + 1)}{2} \prod_{j=1}^{i-1} s_j \right) \right],$$

where the argument of the exponential is written in such a way to ensure that each $s_i = -1$ does not contribute, and each $s_i = 1$ makes a contribution of

$$\frac{\theta}{2}\prod_{j=1}^{i-1} s_j = (-1)^{n_i}\frac{\theta}{2},$$

where n_i is the number of negative signals that precede the element i.

We can simplify the expression for the matrix if we note that

$$\begin{aligned}\sum_{i=1}^{p}\frac{(s_i+1)}{2}\prod_{j=1}^{i-1} s_j &= \frac{1}{2}\left[\left(\sum_{i=1}^{p}\prod_{j=1}^{i} s_j\right)+1+\left(\sum_{i=2}^{p}\prod_{j=1}^{i-1} s_j\right)\right]\\ &= \frac{1}{2}\left[\left(\sum_{i=1}^{p}\prod_{j=1}^{i} s_j\right)+1+\left(\sum_{i=1}^{p-1}\prod_{j=1}^{i} s_j\right)\right],\end{aligned}$$

and that, for $\{s_j\} \in \Lambda^{p\pm}$, $\pm 1 = \prod_{j=1}^{p} s_j$. Then we can write

$$\sum_{i=1}^{p}\frac{(s_i+1)}{2}\prod_{j=1}^{i-1} s_j = \sum_{i=1}^{p}\prod_{j=1}^{i} s_j$$

for $\{s_i\} \in \Lambda^{p+}$ and

$$\sum_{i=1}^{p}\frac{(s_i+1)}{2}\prod_{j=1}^{i-1} s_j = \frac{1}{2}\left[2\left(\sum_{i=1}^{p}\prod_{j=1}^{i} s_j\right)+2\right] = 1+\sum_{i=1}^{p}\prod_{j=1}^{i} s_j$$

for $\{s_i\} \in \Lambda^{p-}$.

The discussion above motivates the proof of the following proposition.

Proposition 1. Consider the one-dimensional Ising model, of period p, with periodic boundary conditions. The matrix $T^{(p)}$, defined by the product of transfer matrices $T^{(p)} = T_1 T_2 \cdots T_p$, has its entries given by

$$T_{11}^{(p)} = \sum_{\{s_i\}\in\Lambda^{p+}}\left(\prod_{i=1}^{p}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{p}\prod_{j=1}^{i} s_j\right],$$

$$T_{12}^{(p)} = \sum_{\{s_i\}\in\Lambda^{p-}}\left(\prod_{i=1}^{p}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{p}\prod_{j=1}^{i} s_j\right)\right].$$

The other entries $T_{22}^{(p)}$ and $T_{21}^{(p)}$ can be obtained by the complex conjugates of $T_{11}^{(p)}$ and $T_{12}^{(p)}$, respectively.

Proof. The proof is made by induction. For $p=2$, we have $\Lambda^{2+}=\{(+1,+1),(-1,-1)\}$, in such a way that

$$T_{11}^{(2)}=(\tau_1\tau_2)^{1/2}e^{i\theta}+(\tau_1\tau_2)^{-1/2}=\sum_{\{s_i\}\in\Lambda^{2+}}\left(\prod_{i=1}^{2}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{2}\prod_{j=1}^{i}s_j\right],$$

$$T_{11}^{(2)}=\tau_1^{1/2}\tau_2^{-1/2}e^{i\theta/2}+\tau_1^{-1/2}\tau_2^{1/2}e^{-i\theta/2}=\sum_{\{s_i\}\in\Lambda^{2-}}\left(\prod_{i=1}^{2}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{2}\prod_{j=1}^{i}s_j\right)\right],$$

and the proposition is valid for $p=2$. Suppose that it is valid for some $p=k$. For $p=k+1$ we have

$$T^{(k+1)}=T^{(p)}T_{k+1}=\begin{pmatrix}T_{11}^{(k)} & T_{12}^{(k)}\\ T_{21}^{(k)} & T_{22}^{(k)}\end{pmatrix}\begin{pmatrix}\tau_{k+1}^{1/2}e^{i\theta/2} & \tau_{k+1}^{-1/2}\\ \tau_{k+1}^{-1/2} & \tau_{k+1}^{1/2}e^{-i\theta/2}\end{pmatrix}. \tag{62}$$

By the induction hypothesis,

$$T_{11}^{(k+1)}=\sum_{\{s_i\}\in\Lambda^{k+}}\left(\prod_{i=1}^{k}\tau_i^{s_i}\right)^{1/2}\tau_{k+1}^{1/2}\exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{k}\prod_{j=1}^{i}s_j\right)\right]$$
$$+\sum_{\{s_i\}\in\Lambda^{k-}}\left(\prod_{i=1}^{k}\tau_i^{s_i}\right)^{1/2}\tau_{k+1}^{-1/2}\exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{k}\prod_{j=1}^{i}s_j\right)\right].$$

We can write $1=\prod_{j=1}^{k+1}s_j$ whenever $\{s_i\}_{i=1}^{k}\in\Lambda^{k+}$ and $s_{k+1}=1$ or $\{s_i\}_{i=1}^{k}\in\Lambda^{k-}$ and $s_{k+1}=-1$. Therefore,

$$T_{11}^{(k+1)}=\sum_{\substack{\{s_i\}\in\Lambda^{k+}\\ s_{k+1}=1}}\left(\prod_{i=1}^{k+1}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{k+1}\prod_{j=1}^{i}s_j\right]$$
$$+\sum_{\substack{\{s_i\}\in\Lambda^{k-}\\ s_{k+1}=-1}}\left(\prod_{i=1}^{k+1}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{k+1}\prod_{j=1}^{i}s_j\right].$$

In fact, the two summations cover the whole set of sequences $\Lambda^{(k+1)+}$, and we have

$$T_{11}^{(k+1)}=\sum_{\{s_i\}\in\Lambda^{(k+1)+}}\left(\prod_{i=1}^{k+1}\tau_i^{s_i}\right)^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{k+1}\prod_{j=1}^{i}s_j\right].$$

Analogously, for the other matrix element,

$$T_{12}^{(k+1)}=\sum_{\{s_i\}\in\Lambda^{k+}}\left(\prod_{i=1}^{k}\tau_i^{s_i}\right)^{1/2}\tau_{k+1}^{-1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{k}\prod_{j=1}^{i}s_j\right]$$
$$+\sum_{\{s_i\}\in\Lambda^{k-}}\left(\prod_{i=1}^{k}\tau_i^{s_i}\right)^{1/2}\tau_{k+1}^{1/2}\exp\left[\frac{i\theta}{2}\sum_{i=1}^{k}\prod_{j=1}^{i}s_j\right].$$

In order to insert the last term in the summation, one should note that $-1=\prod_{j=1}^{k+1} s_j$ whenever $\{s_i\}_{i=1}^{k} \in \Lambda^{k+}$ and $s_{k+1}=-1$ or $\{s_i\}_{i=1}^{k} \in \Lambda^{k-}$ and $s_{k+1}=1$. Therefore,

$$T_{12}^{(k+1)} = \sum_{\substack{\{s_i\} \in \Lambda^{k+} \\ s_{k+1}=-1}} \left(\prod_{i=1}^{k+1} \tau_i^{s_i}\right)^{1/2} \exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{k+1}\prod_{j=1}^{i} s_j\right)\right]$$

$$+ \sum_{\substack{\{s_i\} \in \Lambda^{k-} \\ s_{k+1}=1}} \left(\prod_{i=1}^{k+1} \tau_i^{s_i}\right)^{1/2} \exp\left[\frac{i\theta}{2}\left(1+\sum_{i=1}^{k+1}\prod_{j=1}^{i} s_j\right)\right].$$

As above, the two summations cover $\Lambda^{(k+1)-}$ and the proof is concluded. ∎

Theorem 3 is a direct consequence of the previous result, since $\mathrm{Tr}(T^{(p)}) = 2\,\mathrm{Re}(T_{11}^{(p)})$.

8. THE STRUCTURE OF GAPS. ANALYSING PARTICULAR CASES

From now on, we will use Theorem 3 to treat several examples of periodic chains. By taking different values of p, we shall observe patterns in the distribution of zeros that will be helpful in determining its general properties.

The cases of period $p=1$ and $p=2$ were already treated in the literature, in refs. 3 and 7 respectively. We will reproduce some of these results with the purpose of getting used to our method.

For constant interaction, we have $\Lambda^{1+}=\{+1\}$ which leads to $\mathrm{Tr}(T_1)=2\tau_1^{1/2}\cos(\theta/2)$. Recalling that $\det(T_1)=\tau_1-\tau_1^{-1}$ we have

$$\cos\phi = \frac{\cos(\theta/2)}{(1-\tau_1^{-2})^{1/2}}. \tag{63}$$

From this expression we see that $\cos(\theta/2)$ is bounded by

$$-2\arccos(1-\tau_1^{-2})^{1/2} < \theta < 2\arccos(1-\tau_1^{-2})^{1/2},$$

where the upper and lower bounds are numbers between 0 and 1. In other words, the zeros do not close in onto the positive real axis, what prevents the existence of phase transition. Since this absence of phase transition at non-zero temperature is characteristic of the one-dimensional ferromagnetic Ising model, one should expect to observe this gap for any period p.

Since the distribution of zeros is uniform in ϕ, we can take the inverse of the equation (63) to obtain the integrated density of zeros

$$I(\theta)=\begin{cases}0, & 0\leqslant\theta\leqslant\theta^{+}\\ \dfrac{1}{\pi}\arccos\left[\dfrac{\cos(\theta/2)}{(1-\tau_1^{-2})^{1/2}}\right], & \theta^{+}<\theta\leqslant\pi.\\ 1-I(1-\theta/2\pi), & \pi<\theta\leqslant 2\pi\end{cases}$$

This function can be differentiated to obtain the results presented in the classical papers of Lee and Yang.

For $p=2$ the set to be considered is $\Lambda^{2+}=\{(+1,+1),(-1,-1)\}$ and the relation between ϕ and θ will be

$$\cos(\phi)=\frac{\cos\theta+(\tau_1\tau_2)^{-1}}{[(1-\tau_1^{-2})(1-\tau_2^{-2})]^{1/2}}.$$

This expression allows us to obtain all the Lee–Yang zeros as a function of θ. For the chain of length $N=2n$ we have the following zeros in the interval $[0,\pi]$

$$\theta_m=\arccos\left[\sqrt{(1-\tau_1^{-2})(1-\tau_2^{-2})}\cos\left(\frac{(2k-1)\pi}{2n}\right)-(\tau_1\tau_2)^{-1}\right],$$

for $1\leqslant m\leqslant n$. The zeros between π and 2π are obtained by the symmetry under reflection on the real axis.

As in the case of constant interaction, the zeros are again bounded by a minimum θ^{+}. However, we have also an upper bound θ^{-}, that is responsible a second gap around $\theta=\pi$. These limit values are obtained by taking $\cos\phi=\pm 1$:

$$\theta^{\pm}=\arccos[\pm\sqrt{(1-\tau_1^{-2})(1-\tau_2^{-2})}-(\tau_1\tau_2)^{-1}].$$

The integrated density of zeros is given by

$$I(\theta)=\begin{cases}0, & 0\leqslant\theta\leqslant\theta^{+}\\ \dfrac{1}{2\pi}\arccos\left[\dfrac{\cos(\theta)+(\tau_1\tau_2)^{-1}}{[(1-\tau_1^{-2})(1-\tau_2^{-2})]^{1/2}}\right], & \theta^{+}\leqslant\theta\leqslant\theta^{-}\\ 1/2, & \theta^{-}\leqslant\theta\leqslant\pi\\ 1-I(1-\theta/2\pi), & \pi<\theta\leqslant 2\pi\end{cases}.$$

We shall now see how the method developed in this work can be used to obtain the gap structure for more complex situations of increasing periods. For $p=3$ we have the general relation:

$$\cos\phi=\frac{\cos\dfrac{3\theta}{2}+[(\tau_1\tau_2)^{-1}+(\tau_2\tau_3)^{-1}+(\tau_3\tau_1)^{-1}]\cos\dfrac{\theta}{2}}{[(1-\tau_1^{-2})(1-\tau_2^{-2})(1-\tau_3^{-2})]^{1/2}}. \tag{64}$$

This equation can be treated as a polynomial equation of order 3 in $\cos\theta/2$,

$$\cos\phi=\frac{4\cos^3\dfrac{\theta}{2}+[(\tau_1\tau_2)^{-1}+(\tau_2\tau_3)^{-1}+(\tau_3\tau_1)^{-1}-3]\cos\dfrac{\theta}{2}}{[(1-\tau_1^{-2})(1-\tau_2^{-2})(1-\tau_3^{-2})]^{1/2}}=P(u).$$

where we have defined the variable $u=\cos\theta/2$. It is interesting to note that

$$P(1)=\frac{1+(\tau_1\tau_2)^{-1}+(\tau_2\tau_3)^{-1}+(\tau_3\tau_1)^{-1}}{[(1-\tau_1^{-2})(1-\tau_2^{-2})(1-\tau_3^{-2})]^{1/2}}>1,$$

for $T\neq 0$. This inequality is responsible for the first gap around $\theta=0$.

Figure 7 presents a sketch of the graph of $P(u)$. Since the set of Lee–Yang zeros becomes dense in $\phi\in[0,\pi]$ when the thermodynamic limit is taken, it is also dense in the inverse image of the interval $[-1,1]$, when the

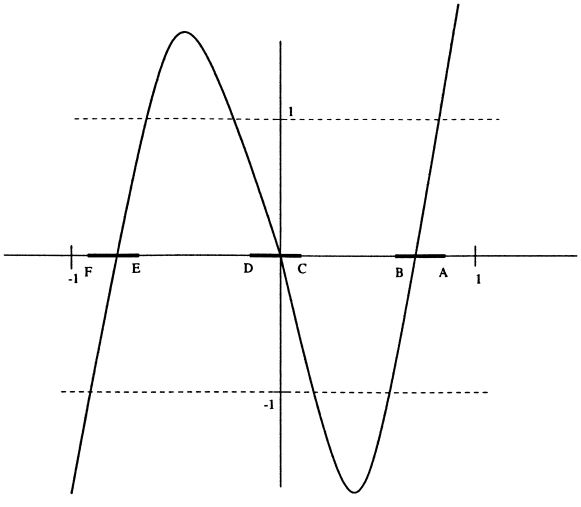


Fig. 7. Sketch of the graph of $P(u)$.

variable θ is considered. The complementary regions are free of zeros, and correspond to the gaps.

We have already explained why the gap around $\theta=0$ appears. The second gap results form the minimum of $P(u)$ that occurs between B and C. Analogously, the maximum between D and E gives rise to the third gap. If we solve the third order polynomial equation $P(u)=1$ we can obtain the values of A, D and E; the solution of $P(u)=-1$ gives us B, C and F.

If we generalise the previous discussion to the case of arbitrary period p, we see that $P'(u)=0$ will be a polynomial equation of order $p-1$, and it will have $p-1$ solutions in the interval $[-1, 1]$. Each solution will be responsible for an extreme value (maximum or minimum) if the function, that will correspond to one gap free of zeros. Moreover, if we consider the gap around $\theta=0$, we obtain that the maximal number of gaps for the periodic chain is equal to its period. We say maximal number because, as we shall see later, certain symmetries can close some of the gaps, since they can only appear when $|P(u)| > 1$ around the points where $P'(u)=0$.

It is interesting to notice that the symmetry under inversion of the magnetic field determines a well-defined parity for $P(u)$. Therefore, in the case of odd period we have only odd powers of u (or factors like $\cos(m\theta/2)$, for $m=1, 3..., p$), whereas for even period only even powers should occur ($\cos m\theta/2$, for $m=0, 2, ..., p$).

The case of period $p=4$ is also interesting, since the results depend only on the solution of a polynomial equation of order $p=$ in $\cos\theta$, allowing us to obtain the exact location of the gaps rather easily. In this case, equation (58) can be written as

$$\cos\phi=\frac{2u^2+\sum_{i=1}^{4}(\tau_i\tau_{i+1})^{-1}u+\sum_{d(i,j)=2}(\tau_i\tau_j)^{-1}+(\prod_{i=1}^{4}\tau_i)^{-1}-1}{[\prod_{i=1}^{4}(1-\tau_i^{-2})]^{1/2}}=P(u),$$

where $d(i, j)$ is the number of edges between the vertices i and j in a closed chain of four vertices and where we redefined the variable u as $u=\cos\theta$ and used $\cos 2\theta=2\cos^2\theta-1$.

Figure 8 sketches $P(u)$ for $u\in[-1, 1]$. Again, the region where the zeros become dense corresponds to $P^{-1}([-1, 1])$. The minimum of the parabolic curve is responsible for the second and fourth gaps. The third gap is the result of $P(-1) > 1$.

To obtain the values of $A^{\pm}$ and $B^{\pm}$, all we have to do is to solve the second order equation

$$2u^2+\left[\sum_{i=1}^{4}(\tau_i\tau_{i+1})^{-1}\right]u+\left[\sum_{d(i,j)=2}(\tau_i\tau_j)^{-1}+\left(\prod_{i=1}^{4}\tau_i\right)^{-1}-1\pm\left(\prod_{i=1}^{4}(1-\tau_i^{-2})\right)^{1/2}\right]=0.$$

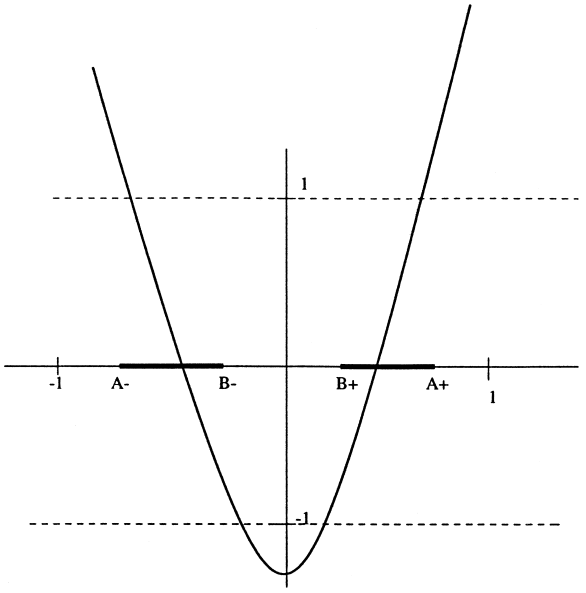


Fig. 8. Sketch of the graph of $P(u)$.

If we consider the case of finite chain of length $N=4n$, the zeros of the partition function will be located at the values

$$\phi=\frac{(k-1/2)\pi}{n}, \qquad k=1, \ldots, n.$$

Therefore, in the y-axis of Figure 8 we have n distinct points in the interval $-1 \leqslant P(u) \leqslant 1$. The inverse image of each of this points leads to two different values of $u=\cos\theta$, which corresponds to four values for θ, each of them in a different region where the zeros become dense. Thus, in the finite case, the number of zeros in each region is exactly one fourth of the total number of zeros. If we take the infinite chain limit, we can label the gaps by the value of the integrated density of zeros (that must be constant inside the gap). Therefore, for $p=4$, the above discussion leads to the following set of labels for the gaps, $\{\frac{m}{4}, m=0, 1, \ldots, 4\}$, where $m=0$ and $m=4$ correspond to the same gap.

For arbitrary period, the analysis is also valid. However, the inverse image of $\cos[(k-1/2)\,\pi/n]$ will be composed of p points $u=\cos(\theta/2)$, distributed along the p dense regions. Therefore, the gaps can be labelled by the values $\{\frac{m}{p}, m=0, 1, \ldots, p\}$.

We shall now analyse the conditions that must be satisfied in order to ensure that each of the gaps does in fact appear in the thermodynamic limit. First,

$$P(1)=\frac{1+[\sum_{i=1}^{4}(\tau_i\tau_{i+1})^{-1}+\sum_{d(i,j)=2}(\tau_i\tau_j)^{-1}+(\prod_{i=1}^{4}\tau_i)^{-1}]}{[\prod_{i=1}^{4}(1-\tau_i^{-2})]^{1/2}}$$

results in

$$P(1) > 1, \qquad T \neq 0, \tag{65}$$

$$P(1) = 1, \qquad T = 0, \tag{66}$$

as it was expected, since the one-dimensional Ising model with short range interactions is not expected to exhibit a phase transition for finite temperature. Regarding the gap around $\theta=\pi$,

$$P(-1)=\frac{1+[-\sum_{i=1}^{4}(\tau_i\tau_{i+1})^{-1}+\sum_{d(i,j)=2}(\tau_i\tau_j)^{-1}+(\prod_{i=1}^{4}\tau_i)^{-1}]}{[\prod_{i=1}^{4}(1-\tau_i^{-2})]^{1/2}}.$$

It is straightforward to show that $P(-1)=1$ when $\tau_1=\tau_2=\tau_3=\tau_4$. However, it is not only in this rather trivial situation that the third gap closes. As we have said earlier, certain symmetries can close some of the gaps without reducing the period. Let us, for instance, consider the case where $\tau_1=\tau_2=x^{-1}$ and $\tau_3=\tau_4=y^{-1}$. Although the period is still $p=4$, we have now

$$P(-1)=\frac{1+x^2y^2-x^2-y^2}{(1-x^2)(1-y^2)}=1,$$

which means that the third gap closes (see Figure 9).

The fact that symmetries can close some of the gaps must be considered in the case of greater period, and also in the case of aperiodic chains, where the sequence of interactions is given by a substitution rule (Thue-Morse, Fibonacci, etc.).[7]

It remains to study the value of $P(u)$ at the vertex of the parabolic curve, that we denote by $P(u_v)$. Whenever $P(u_v) < -1$, the second and fourth gap appear. We have

$$P(u_v)=\frac{-[\sum_{i=1}^{4}(\tau_i\tau_{i+1})^{-1}]^2+8[\sum_{d(i,j)=2}(\tau_i\tau_j)^{-1}+(\prod_{i=1}^{4}\tau_i)^{-1}-1]}{8[\prod_{i=1}^{4}(1-\tau_i^{-2})]^{1/2}}.$$

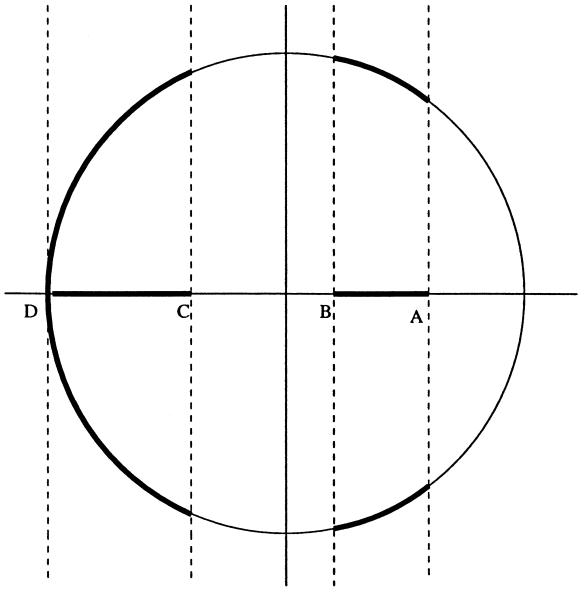


Fig. 9. Unitary circle $|z|=1$.

When $\tau_1=\tau_2=\tau_3=\tau_4=x^{-1}$ we have

$$P(u_v)=\frac{-16x^4+8(2x^2+x^4-1)}{8(1-x^2)^2}=-1. \tag{67}$$

The gaps also close when we reduce the period of the chain to $p=2$ by taking $\tau_1=\tau_3=x^{-1}$ and $\tau_2=\tau_4=y^{-1}$:

$$P(u_v)=\frac{-8(1-x^2-y^2+x^2y^2)}{8(1-x^2)(1-y^2)}=-1. \tag{68}$$

9. CONCLUSIONS

We have studied the distribution of the Lee–Yang zeros for the Cayley Tree, with interactions that vary in a periodic or aperiodic way (but given by sequences generated by substitutions) along the generations. Our main interest was to determine the circumstances under which the set of Lee–Yang zeros become dense over the unit circle. The importance of this fact is that, if the zeros are dense around $|z|=1$, some of the thermodynamic functions cannot be analytically continued from $|z|<1$ to $|z|>1$. For

instance, one can study the behaviour of the magnetisation at the origin when the zeros become dense. For period $p=2$ and order $d=2$, we have proved that a phase transition occurs only for $\Lambda(\rho_a, \rho_b) \geqslant 1$. In the complementary region, the absence of phase transition is explicitly shown.

For generic period p and order d, the properties of the distribution of zeros are derived from the Liapunov exponent of the related dynamical system and all one has to do is evaluate the generalised function $\Lambda^{(d)}(\rho_1, \rho_2, \cdots, \rho_p)$, whose logarithm provides a lower bound for the Liapunov exponent. In the case where $\Lambda^{(d)}(\rho_1, \rho_2, \cdots, \rho_p)$ is greater or equal than one, we have a dense set of zeros. Otherwise, the distributions has a gap around $|z|=1$ and no phase transition should occur.

The aperiodic case, where the interactions are derived from a sequence generated by a substitution rule in a finite alphabet, is rather interesting, since the occurrence frequency of each of the interactions can be calculated explicitly. We have proved that the region where the zeros become dense depends only on the value of each of the interactions and their frequencies. We were also able to obtain results for the Fibonacci and the Thue–Morse sequences, but one can employ our ideas for any substitutional sequence (Rudin–Shapiro, etc).

In this work, we were only concerned about the gap around $\theta=0$ for the Cayley Tree, and the structure of gaps that may appear for periodic interactions was not analysed. The fact that a periodic sequence of interactions leads to a sequence of gaps in the unit circle of the fugacity variable is well-known for the one-dimensional lattice. In this case, we were able to obtain a general treatment for the gap structure for arbitrary period p. From this treatment, one can obtain the number of gaps for each sequence of interactions and locate them in the unit circle. The conjunction of the results from the two parts of this work might be used as the starting point to obtain the general gap structure for the rooted Cayley Tree (and for other lattices with properties not to different from the one-dimensional lattice), although the absence of transfer matrices formalism may introduce some difficulties in the treatment.

APPENDIX. SUBSTITUTION SEQUENCES

Let $A=\{0, 1, ..., s-1\}$ be a finite set with $\text{card}A=s$. $A^*=\bigcup_{k\geqslant 1} A^k$ denotes the set of all finite words over the alphabet A. We consider the set $A^{\mathbb{N}}$ which consists in sequences $x=\{x_n\}_{n\geqslant 0}$ with components in A. $A^{\mathbb{N}}$ is endowed with the topology defined by the metric

$$d(x, y)=\begin{cases}\exp(-\min\{k \geqslant 0, x_k \neq y_k\}), & \text{if} \quad x \neq y \\ 0, & \text{if} \quad x=y\end{cases}. \tag{69}$$

It is important to note that $A^{\mathbb{N}}$ is complete with the metric above. We define on $A^{\mathbb{N}}$ the one-sided shift transformation by $(Tx)_k = x_{k+1}$. Clearly, T is continuous and surjective.

A substitution ρ on A is a map from A to A^* which associates to the letter $i \in A$, $0 \leqslant i < s$ the word $\rho(i)$. Any substitution ρ induces a map from A^* to A^*, which associates to the word $B = b_0 \cdots b_n$ the word $\rho(B) = \rho(b_o) \cdots \rho(b_n)$. Analogously, we define a map from $A^{\mathbb{N}}$ to $A^{\mathbb{N}}$ by $\rho(x) = \rho(x_0)\, \rho(x_1) \cdots$.

Since we are interested in fixed points of ρ, we should note the following result

Proposition 2 (See ref. 12). Let ρ be a substitution rule such that, for every $\alpha \in A$, $|\rho^n(\alpha)|$ goes to infinity. Then, there exists $u \in A^{\mathbb{N}}$ fixed point of ρ^k, for some $k \geqslant 1$.

We can find α and a positive k such that $\rho^k(\alpha)$ begins by α (otherwise, the alphabet would not be finite). Let x be an arbitrary sequence which begins by α. Then, $\rho^{kn}(x)$ begins by $\rho^{kn}(\alpha)$, so that $\rho^{kn}(x)$ e $\rho^{kn+kp}(x)$ begins by the same word, whose length goes to infinity. $\{\rho^{kn}\}$ is a Cauchy sequence in $A^{\mathbb{N}}$, and converges to a sequence satisfying $u = \rho^k(u)$ and beginning by α. We can obtain this fixed point of ρ^k by iterating the substitution ρ^k on α.

From now on, we assume that for all $\alpha \in A$, $\lim_{n \to \infty} |\rho^n(\alpha)| = \infty$. Moreover, there exists a letter, which we denote by 0, such that $\rho(0)$ begins by 0.

Let us denote by u the fixed point of ρ, obtained by $u = \rho^\infty(0)$. We shall consider only the letters of A which actually appear in u.

In order to prepare for the Perron–Frobenius Theorem, we should consider the following definition.

Definition 1. A substitution ρ is said to be primitive if there exists k such that $\rho^k(\alpha)$ contains β, for all α and β.

If B and C are words in A^*, we denote by $L_C(B)$ the occurrence number of C in B. In particular, if $i \in A$, $L_i(B)$ is the number of i occurring in B.

With this notation, we define the ρ-matrix $M = M(\rho)$ whose entries are $M_{ij} = L_i(\rho(j))$. For instance, the Fibonacci sequence, defined in the alphabet $\{a, b\}$ by

$$\rho(a) = b, \qquad \rho(b) = ba, \tag{70}$$

has the substitution matrix M given in (52).

Since $M_{ij}^k = L_i(\rho^k(j))$, we can say that ρ is primitive if and only if M is primitive, which means that M^k is strictly positive for some k. Therefore, for any primitive ρ, we can apply the Perron–Frobenius Theorem to the substitution matrix $M(\rho)$.

Theorem 4 (See ref. 12). Let M be a primitive positive matrix. Then

1. M admits a positive eigenvalue θ, such that $\theta > |\lambda|$ for any other eigenvalue λ of M.
2. There exists a strictly positive eigenvector corresponding to θ.
3. θ is a simple eigenvalue.

Let ρ be any primitive substitution on A. The following propositions are corollaries of the Perron–Frobenius Theorem.

Proposition 3 (See ref. 12). For every $\alpha \in A$, the sequence $\left\{\frac{L(\rho^n(\alpha))}{\theta^n}\right\}_{n \geq 1}$ converges to a strictly positive eigenvector corresponding to θ.

Since θ is a simple eigenvalue, we may decompose M into the sum $M = \theta P_\theta + N$, where P_θ is some projection onto the one-dimensional space $\ker(M - \theta I)$, and N is an operator satisfying $NP_\theta = P_\theta N = 0$. Therefore, we have $M^n = \theta^n P_\theta + N^n$, or

$$\frac{M^n}{\theta^n} = P_\theta + \frac{N^n}{\theta^n}. \tag{71}$$

Since θ is the dominant eigenvalue, the last term in the right hand side goes to zero and $\lim_{n\to\infty} \frac{M^n}{\theta^n} = P_\theta$. Using $\frac{L(\rho^n(\alpha))}{\theta^n} = \frac{M^n L(\alpha)}{\theta^n}$, we have

$$\lim_{n\to\infty} \frac{L(\rho^n(\alpha))}{\theta^n} = P_\theta(L(\alpha)). \tag{72}$$

Since $L(\alpha)$ has all its components equal to zero, except for the α-component, which is equal to 1, it follows that its projection is a strictly positive eigenvector corresponding to θ.

The next result provides a way to calculate the occurrence frequency of each of the letter in the limit sequence.

Proposition 4 (See ref. 12). Let $\alpha, j \in A$. Then

$$\lim_{n\to\infty} \frac{L_j(\rho^n(\alpha))}{|\rho^n(\alpha)|} = v_j > 0 \tag{73}$$

and this limit is independent of α.

We observe that

$$\lim_{n\to\infty}\frac{L(\rho^n(\alpha))}{|\rho^n(\alpha)|}=\lim_{n\to\infty}\frac{L(\rho^n(\alpha))}{\langle L(\rho^n(\alpha)),I\rangle}=\lim_{n\to\infty}\frac{L(\rho^n(\alpha))/\theta^n}{\langle L(\rho^n(\alpha))/\theta^n,I\rangle}=\frac{w(\alpha)}{\langle w(\alpha),I\rangle}, \quad (74)$$

where $w(\alpha)=P_\theta L(\alpha)$ is the positive eigenvector associated to θ, obtained in the last proposition. One can notice that $v=(v_j)$ is normalised by, $\sum_{j=0}^{s-1} v_j=1$. Therefore, and since θ is a simple eigenvalue, it follows that the number v_j are positive and independent of α.

As a result, all one has to do in order to obtain the occurrence frequency of each of the letter in the final chain is to calculate the positive eigenvector associated to the maximal eigenvalue of the substitution matrix.

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