Journal of Statistical Physics, Vol. 78, Nos. 1/2, 1995

Partition Function Zeros for Aperiodic Systems

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Received October 25, 1993; final May 17, 1994

The study of zeros of partition functions, initiated by Yang and Lee, provides an important qualitative and quantitative tool in the study of critical phenomena. This has frequently been used for periodic as well as hierarchical lattices. Here, we consider magnetic field and temperature zeros of Ising model partition functions on several aperiodic structures. In 1D, we analyze aperiodic chains obtained from substitution rules, the most prominent example being the Fibonacci chain. In 2D, we focus on the tenfold symmetric triangular tiling which allows efficient numerical treatment by means of corner transfer matrices.

KEY WORDS: Ising model; Lee–Yang zeros; edge singularities; nonperiodic systems; phase transitions; gap labeling.

1. INTRODUCTION

The study of critical phenomena by means of discrete spin systems, initiated by Lenz and Ising,[1] finally came of age in Onsager's spectacular solution of the 2D field-free Ising model.[2] He could show that the 2D Ising model on the square lattice with ferromagnetic nearest-neighbor interaction exhibits an order–disorder phase transition of second order at finite temperature with the magnetization as order parameter.

The investigation of many other spin systems followed, as did the consideration of Ising-type models on other lattices and graphs. Some cases can still be solved exactly,[3] but this is an exception. Consequently, one needs complementary methods to tackle questions like existence and location of critical points and estimation of critical exponents, especially in

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0022-4715/95/0100-0285$07.50/0

higher dimensions. One such technique is provided by the work of Lee and Yang,[4,5] who investigated the distribution of partition function zeros in the complex plane, i.e., field variables or fugacity were treated as a complex parameter. Later, also the zeros in the complex temperature variable were studied for various systems.[6–11] These provide information not only about the location of phase boundaries, but also about critical exponents; see, e.g., ref. 10, where mainly hierarchical lattices are considered. For those, the zero patterns form fractal structures known as Julia sets, whereas they are usually expected to lie on simple curves for regular lattices, at least in the isotropic case. It has been shown[12,13] that for anisotropic Ising models on two-dimensional regular lattices the temperature zeros generically fill areas in the complex plane.

But what does "simple curves" mean? As we will show, already the Ising model on a modulated structure in 1D can result in magnetic field zeros which *do* lie on a simple curve, but occupy only a Cantor-like portion of it—even in the thermodynamic limit! This shows that fractal distributions of Lee–Yang zeros do *not* require hierarchical graphs. This also gives new (and possibly interesting) situations where edge singularities may contain substantial information about the system, but we will not discuss that here.

Although the corresponding phenomenon in 2D does not typically show up (or at least not that we could conclude so), the investigation of partition function zeros for spin systems on nonperiodic graphs with inflation/deflation symmetry might fill the gap between the relatively well-studied cases of lattices and hierarchical graphs. This is why we discuss the Ising model on certain quasiperiodic graphs. In 2D, we present magnetic field and temperature zeros for a nonperiodic Ising model on the so-called triangle tiling. Since exact results seem rather hard to obtain, we have chosen this example because it allows precise numerical treatment up to relatively large patches by means of corner transfer matrices.

2. NONPERIODIC 1D ISING MODEL

Let us consider a one-dimensional chain of N Ising spins $\sigma_j \in \{\pm 1\}$, $j = 1, 2, ..., N$, with periodic boundary conditions (i.e., $\sigma_{N+1} = \sigma_1$). The energy of a configuration $\sigma = (\sigma_1, \sigma_2, ..., \sigma_N)$ is given by

$$E(\sigma) = -\sum_{j=1}^{N} J_{j,j+1}\sigma_j\sigma_{j+1} + H_j\sigma_j \tag{2.1}$$

Here, we concentrate on systems where the coupling constants $J_{j,j+1}$ can only take two different values $J_{j,j+1} \in \{J_a, J_b\}$ and where the magnetic field is constant, i.e., $H_j \equiv H$. The actual distribution of the two coupling constants J_a and J_b along the chain is determined by an infinite word in the letters a and b which is obtained as the unique limit of certain two-letter substitution rules.[14] In fact, we restrict ourselves to the Fibonacci case, which corresponds to the substitution rule

$$S\colon\quad \begin{array}{l} a \to b \\ b \to ba \end{array} \tag{2.2}$$

The length of the word $w_n = S(w_{n-1})$ obtained by n iterations from the initial word $w_0 = a$ is f_{n+1}, where the Fibonacci numbers f_n are defined by

$$f_0 = 0, \qquad f_1 = 1, \qquad f_{n+1} = f_n + f_{n-1} \tag{2.3}$$

Let us introduce the following notation:

$$K_a = \frac{J_a}{k_B T}, \qquad K_b = \frac{J_b}{k_B T}, \qquad h = \frac{H}{k_B T} \tag{2.4}$$

and

$$z_a = \exp(2K_a), \qquad z_b = \exp(2K_b), \qquad w = \exp(2h) \tag{2.5}$$

The two elementary transfer matrices[3] T_a and T_b now read

$$T_{a,b} = (w \cdot z_{a,b})^{-1/2} \begin{pmatrix} w \cdot z_{a,b} & \sqrt{w} \\ \sqrt{w} & z_{a,b} \end{pmatrix} = (w \cdot z_{a,b})^{-1/2}\, \tilde{T}_{a,b} \tag{2.6}$$

and, in general, do *not* commute with each other.

The recursive definition of the sequence gives rise to a recurrence formula for the transfer matrices

$$T_0 = T_a, \qquad T_1 = T_b, \qquad T_{n+1} = T_n \cdot T_{n-1} \tag{2.7}$$

where T_n denotes the transfer matrix of the chain that corresponds to the nth iteration step. Hence the partition function $Z_n(z_a, z_b, w) = \mathrm{tr}(T_n)$ is essentially (i.e., up to an overall factor) a polynomial in its three variables. It is also possible to write down a recurrence relation for the partition function itself; see refs. 14–16 for details. In this way, it is really easy to generate the partition function for very large systems exactly (e.g., by means of algebraic manipulation packages). Our problem at hand has thus been reduced to the task of computing the roots of a polynomial.

Let us look at the pattern of zeros of the partition functions $Z_n(z_a, z_b, w)$ in the field variable w. If both couplings are ferromagnetic

($z_a \geqslant 1$, $z_b \geqslant 1$), the zeros lie on the unit circle.[17] Similarly, for purely antiferromagnetic coupling ($z_a \leqslant 1$, $z_b \leqslant 1$), they are on the negative real axis (i.e., the zeros in the variable $w^{1/2} = e^h$ lie on the imaginary axis), whereas the "mixed" case turns out to be complicated and will not be discussed here.

For simplicity, we will from now on stick to the purely *ferromagnetic* regime. If the chain were periodic, the zeros would follow a well-known distribution on the unit circle (they can be calculated analytically[18,19]). In the thermodynamic limit, they fill a connected part of the circle densely (though not uniformly if $0 < T < \infty$): a gap only remains near the point $(1, 0)$ on the real axis, with an opening angle depending on T; compare ref. 19 for details. Near the gap one finds the famous Lee–Yang edge singularity of the density of zeros[5] with exponent $-1/2$.[20] The gap closes only for $T = 0$, which means that we do not have a phase transition at finite temperature ($T > 0$). One might perhaps expect the very same (and simple) situation in the Fibonacci case, but the latter is always good for a surprise.

In Fig. 1, we show the location of the zeros of $Z_n(z_a, z_b, w)$ in the complex w plane for ferromagnetic couplings $z_a = 3/2$, $z_b = 100$ (which corresponds to $K_a \approx 0.203$ and $K_b \approx 2.306$) and $n = 8, 9, 10$. As expected, the zeros are clearly located on the unit circle, and there is still a large gap near (1,0), as it must be because we still cannot have a phase transition at finite temperature. However, an *additional* gap structure in the distribution of the zeros on the unit circle is apparent. It turns out that this gap structure does not depend on the actual values of the coupling constants (as long as they are still ferromagnetic), just the gap widths change and the gaps vanish if z_a and z_b become equal, which of course corresponds to the periodic case. The large difference between the two couplings used in our pictures was chosen to show the effect clearly—for a small difference one might miss it, though it is still there! Consequently, as can also be guessed from Fig. 1, there should be a whole hierarchy of edge singularities (the limiting set of zeros consists of edges only, so to say). The calculation of their exponents would be an interesting task, but is beyond the scope of this article.

Let us rather take a closer look at the gaps themselves. In Fig. 2, we present the integrated density of the zeros on the unit circle (i.e., the integrated density of their angles (in units of 2π) with respect to the real axis) for the same set of parameter values as in Fig. 1. It turns out that this has exactly the structure which one would expect from the general gap labeling theorem of Bellissard and coworkers[21,22,14] which originally

[5] Note the similarity to the van Hove singularity of the electronic density of states at the band edges in 1D.

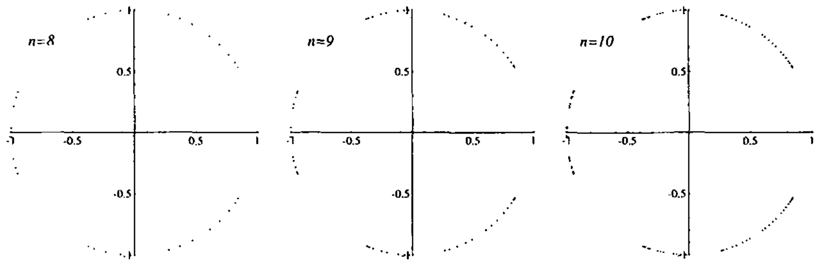

Fig. 1. Zeros of the partition function $Z_n(z_a, z_b, w)$ of the Fibonacci Ising chain in the field variable $w = \exp(2h)$ for $z_a = 3/2$, $z_b = 100$, and $n = 8, 9, 10$.

applies to the integrated density of states (IDOS) of energy spectra of certain discrete Hamiltonians. There, the limit set of the IDOS values at the gaps has the form (see ref. 14 and references therein)

$$\mathscr{G} = \left\{ \frac{\mu}{\tau} + \frac{\nu}{\tau^2} \,\middle|\, \mu, \nu \in \mathbb{Z} \right\} \cap [0, 1] \tag{2.8}$$

for the Fibonacci case, where $\tau = (1 + \sqrt{5})/2$ is the golden ratio. The widest gaps in Fig. 2 have been labeled with the corresponding indices (μ, ν), which for the finite system belong to the rational values

$$(\mu, \nu): \quad \frac{\mu f_n + \nu f_{n-1}}{f_{n+1}} \xrightarrow{n \to \infty} \frac{\mu}{\tau} + \frac{\nu}{\tau^2} \tag{2.9}$$

of the integrated density. Note that any two successive Fibonacci numbers f_{n-1} and f_n are coprime, hence every integer can be written as a linear combination of them with integral coefficients. Actually, since $\tau^2 = \tau + 1$, one could alternatively label the gaps for the Fibonacci case by a single algebraic integer in the ring $\mathbb{Z}[\tau]$,[22] but we prefer to use the above notation, which immediately generalizes to a large class of substitution

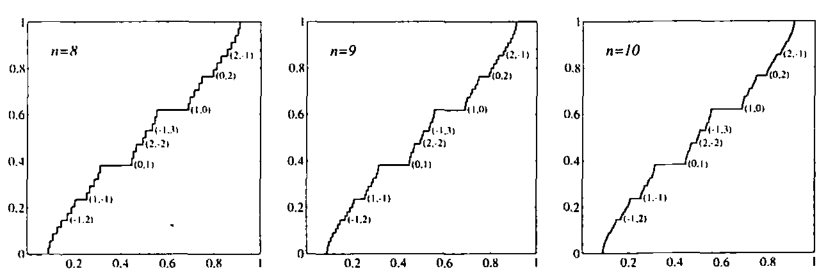

Fig. 2. Integrated density of the zeros in Fig. 1 on the unit circle. The corresponding gap labels [see Eq. (2.9)] for the widest gaps are also shown.

rules.[14] Furthermore, (2.9) shows the relation to the gaps of the periodic approximants more transparently. Generically, it appears that at all the "allowed" values one actually observes gaps in the density distribution, i.e., "all gaps are open." The obvious symmetry in the pictures which relates the gaps with labels (μ, ν) and $(1-\mu, 1-\nu)$ stems from the reflection symmetry of the zero pattern with respect to the real axis which corresponds to a change of the sign in the magnetic field h.

Admittedly, we did not present a rigorous argument which explains why the gap labeling theorem for the IDOS of one-dimensional Schödinger operators[21,22,14] describes the distributions of our partition function zeros on the unit circle. However, the agreement is certainly convincing and suggests that one might think of the zeros (or rather of their arguments) as the eigenvalues of a Schrödinger-type operator. This is also one relatively easy way to prove the Lee–Yang circle theorem (or the corresponding "line theorem" in the antiferromagnetic case) for the periodic 1D Ising model. In this context, we also mention an old idea of Hilbert's, namely the possible connection between the imaginary parts of the (nontrivial) zeros of the Riemann ζ-function and the eigenvalues of a—so far unknown—Hermitian Hamiltonian. This has recently also been linked to some typical aspects of quantum chaos; see ref. 23 and references therein.

3. ISING MODEL ON THE TRIANGLE TILING

The 1D case was presented for two main reasons. On the one hand, calculations are either possible analytically or can be made rigorous. On the other hand, a new phenomenon—the appearance of gaps—could be seen.

Nevertheless, investigations of Ising models on graphs of higher dimension are in order. If one is not interested in approximative calculations (which we are not), one encounters true difficulties on the nonperiodic ground. Even the existence of local inflation/deflation symmetry does not seem to allow exact renormalization schemes for electronic models,[24,25] and we were not able to find one for Ising-type models either.

So, the best thing one can then do is the exact calculation of the partition sum for finite patches, followed by a numerical approach of the thermodynamic limit. Even this is a difficult task which requires a good choice of the graph, i.e., the nonperiodic tiling. From our experience with Ising quantum chains in 1D[26]—which can be seen as anisotropic limits of 2D classical systems—we decided to take a quasiperiodic example in order to stay free of difficult effects caused by fluctuations (which, however, may yield new physics; see, e.g., refs. 27 and 28).

The triangle tiling developed in Tübingen[29–31] has the advantage that we can start from a patch with decagonal boundary that is—in a natural

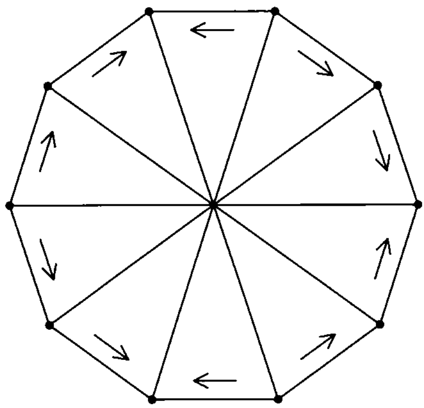

Fig. 3. Initial decagonal patch of the Tübingen triangle tiling.

way—partitioned into *sectors*, each covering an angle of $2\pi/10$; see Fig. 3. This tiling is quasiperiodic and can be generated by successive substitution or inflation[6] as well as by the standard projection technique; for details see ref. 30. It consists of two golden triangles (of two orientations each) (see Fig. 4), and thus has two types of edges with length ratio $\tau = (1+\sqrt{5})/2$. We identify them with two different bonds and attach different couplings to them. In our present context, we consider the cartwheel tiling which is obtained from the patch of Fig. 3 by repeated application of the inflation rule of Fig. 4 and which does preserve the sectoral structure in each step; see Fig. 5.

This structure suggests the use of corner transfer matrices (CTMs) for the sectors[3] to calculate the partition sum and the magnetization at the center of the patch. However, the patch is not a repetition of ten equal sectors; therefore we cannot reduce the problem to the CTM of one single sector. On the other hand, the CTMs of sectors of opposite orientation (indicated by the arrow in the initial patch) are the transposed matrices of each other. Giving half weight to all bonds and all magnetic field terms of single spins on the boundaries of the sector, we can obtain the partition function as

$$Z = \mathrm{tr}((M^2 M' M^2) \cdot (M^2 M' M^2)') \tag{3.1}$$

Here, M is the CTM of a single sector and we have used the symmetry of Fig. 3 (and of all patches obtained from it by successive inflation) under reflection in the horizontal axis. Equation (3.1) can then be evaluated again by algebraic manipulation packages.

[6] This process is normally called *deflation* in the physical literature and *inflation* in the mathematical literature. We use the latter convention here.

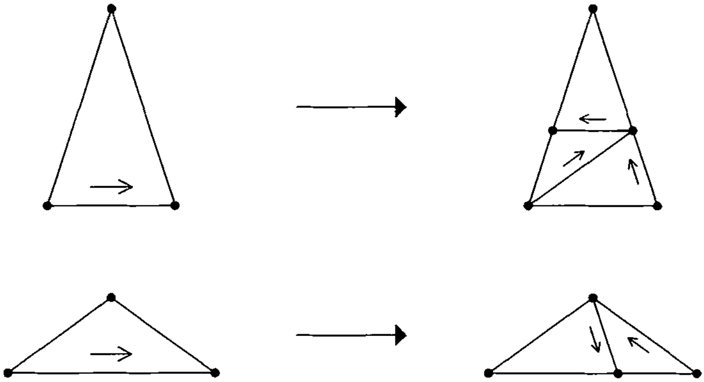

Fig. 4. Inflation rules for the Tübingen triangle tiling.

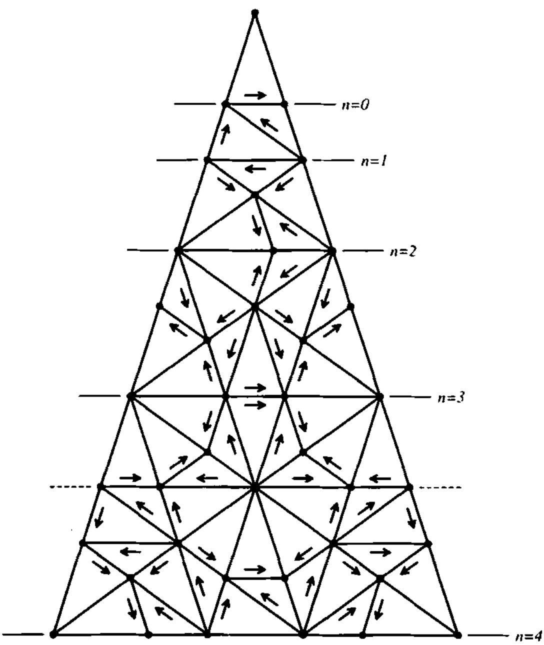

Fig. 5. One sector of Fig. 3 after n inflation steps (see Fig. 4) for $n \leqslant 4$. The dashed line indicates a sector that also leads to a patch with decagonal boundary, which, however, is not obtained by entire inflation steps from the initial patch shown in Fig. 3.

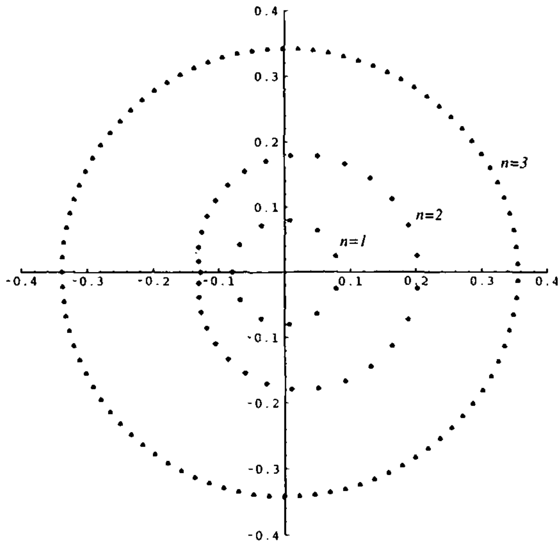

Fig. 6. Zeros of the partition function $Z_n(4, 4, w)$ (fixed boundary conditions) in the field variable w for $n = 1, 2, 3$.

In what follows, we use the same notation as in the Fibonacci case above, but with indices s (for short) and l (for long) in place of a and b. In particular, we also assume that the magnetic field is uniform. Here, $Z_n(z_s, z_l, w)$ now denotes the partition function of the Ising model on the patch which is obtained by n inflation steps (see Fig. 4) from the initial decagonal patch shown in Fig. 3 (which corresponds to $n = 0$). It is impossible to define periodic boundary conditions on our tiling without destroying the tenfold symmetry[7] and the sector structure; therefore we either use fixed boundary conditions (i.e., all spins on the decagonal boundary of the patch are frozen to be $+1$) or free boundary conditions (i.e., we sum over all values of the boundary spins).

For fixed boundary conditions, the zeros of the partition function $Z_n(z_s, z_l, w)$ (for finite n) in the field variable w are no longer located on the unit circle, as this case (in contrast to the free boundary case) is not covered by the circle theorem of Lee and Yang.[5] This is clearly seen in Fig. 6, which shows the locations of the zeros in the complex w plane for couplings $z_s = z_l = 4$ and three different patch sizes. The picture is somewhat surprising,-as the finite-size effects on the absolute values of the zeros are quite large. Nevertheless, it is plausible (though certainly not obvious from Fig. 6) that the zeros approach the unit circle in the thermodynamic

[7] See ref. 30 for details on the symmetry concept needed here.

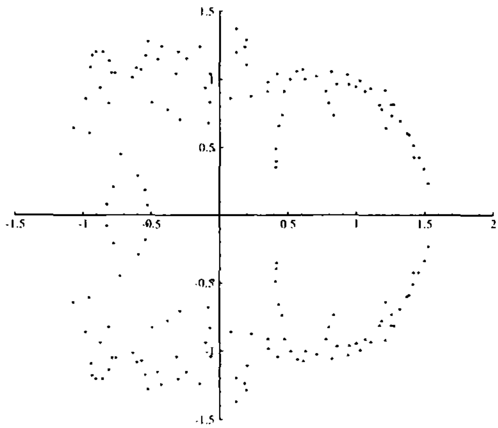

Fig. 7. Zeros of the partition function $Z_3(z, z, 1)$ (fixed boundary conditions) for the "isotropic" zero-field case (equal coupling for long and short bonds) in the temperature variable z.

limit. However, the angular distribution of the zeros is remarkably regular; there is no apparent gap structure as in the one-dimensional case. We also computed the zeros for different couplings z_s and z_l for fixed and free boundary conditions, which show the same behavior.

Let us also look at the zeros in the other variables. Here, we restrict ourselves to the zero-field partition function $Z_n(z_s, z_l, 1)$ and use fixed boundary conditions. For the "isotropic" case $z = z_s = z_l$, the zeros of $Z_3(z, z, 1)$ in the variable z are shown in Fig. 7. Although the distribution of the zeros in the complex z plane is apparently not simple (i.e., the zeros do not appear to lie on simple curves), the zeros close to the real axis contain information about the location of the critical point and, in principle, also about the critical exponents.[32,10] In Table 1, we give the numerical values of the zero closest to the real line with a real part greater than one for the following five choices of (z_s, z_l): $(1, z)$, (z, z^2), (z, z), (z^2, z), and $(z, 1)$, i.e., in addition to the "isotropic" case we look at those cases where

Table I. Partition Function Zero Located Closest to the Real Line and with a Real Part Greater than One, for Vanishing Magnetic Field and Fixed Boundary Conditions

n	$z_s = 1$	$z_s = z_l^2$	$z_s = z_l$	$z_s^2 = z_l$	$z_l = 1$
1	$1.3514 \pm 0.9560i$	$1.2396 \pm 0.2819i$	$1.3249 \pm 0.4315i$	$1.1987 \pm 0.2492i$	$1.4511 \pm 1.3404i$
2	$1.8056 \pm 0.8702i$	$1.3270 \pm 0.2006i$	$1.4709 \pm 0.3238i$	$1.2788 \pm 0.1844i$	$2.4447 \pm 1.3460i$
3	$1.9089 \pm 0.6472i$	$1.3670 \pm 0.1412i$	$1.5249 \pm 0.2322i$	$1.2983 \pm 0.1320i$	$3.0508 \pm 1.1471i$

one of the coupling constants vanishes and where one coupling constant is twice as large as the other.

The approximants for the critical couplings are in good agreement with our values obtained from the behavior of the specific heat and the center spin magnetization of the model (with the exception of $z_l = 1$, where the center spin is isolated), but we omit details here. Let us only remark that the nature of the critical point looks very much like that of the periodic case, though further calculations are needed to confirm that.

4. CONCLUDING REMARKS

The distribution of partition function zeros on the unit circle shows a gap structure for ferromagnetic Ising models on aperiodic chains. Although we have only demonstrated this phenomenon for the ubiquitous Fibonacci chain, one can translate each step to *any* of the other chains obtained by substitution rules—no matter whether one restricts oneself to the two-letter case or not.

The 2D case did not show any apparent gap structure for the magnetic field zeros (and thus resembles the situation of the electronic spectra again). The partition function zeros in the temperature variable do not seem to lie on simple curves, even in the "isotropic" case where the couplings for short and long bonds are identical—more work is to be done to clarify this point. On the other hand, one can clearly see the existence of a phase transition, because the zeros "pinch" the real axis. For given (finite) coupling constants, the critical point has finite T_c.

Now, looking at the limiting cases $z_s = 1$ and $z_l = 1$, one gets the impression that T_c heads to 0, quite similarly as in the case of the square lattice.[3] However, the corresponding graph with one type of bond "switched off" is by no means one-dimensional (or at least not in an obvious way)—wherefore the question arises what this means. To clear this up, one should first treat a model where the location of the critical point can be found exactly, without numerical estimates. This is indeed partially possible for another quasiperiodic tiling, the so-called Labyrinth. An investigation of this phenomenon is more promising there, but we will discuss details elsewhere.[33]

ACKNOWLEDGMENTS

It is a pleasure to thank K. M. Briggs for helpful support in calculating the zeros of large polynomials *correctly*. M.B. is grateful to H.-R. Trebin and the University of Stuttgart for hospitality during the final stage of this work. We also acknowledge support from the Australian Research Council, Deutsche Forschungsgemeinschaft and the EC Human Capital and Mobility Programme.

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