Planar quasiperiodic Ising models
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Abstract

We investigate zero-field Ising models on periodic approximants of planar quasiperiodic tilings by means of partition function zeros and high-temperature expansions. These are obtained by employing a determinant expression for the partition function. The partition function zeros in the complex temperature plane yield precise estimates of the critical temperature of the quasiperiodic model. Concerning the critical behaviour, our results are compatible with Onsager universality, in agreement with the Harris-Luck criterion based on scaling arguments.

Keywords: quasicrystals; Ising model; partition function zeros; phase transition; critical point properties

1. Introduction

The recent, rather controversial discussions about magnetic ordering in quasicrystals, in particular for alloys containing rare earth elements [1, 2], have revived the interest in simple models of magnetic ordering in quasicrystals and their properties. The influence of an aperiodic order on magnetic phase transitions can be understood by heuristic scaling arguments [3, 4] resulting in the Harris-Luck criterion for the relevance of aperiodicity. For one-dimensional aperiodic Ising quantum chains, equivalent to two-dimensional layered Ising models with one-dimensional aperiodicity, exact real-space renormalization techniques can be used that prove the heuristic criterion for a large class of models based on substitution systems [5, 6]. For the classical Ising model defined on two-dimensional quasiperiodic cut-and-project tilings, the criterion predicts that the critical behaviour is the same as for periodic lattices, hence these models belong to the Onsager universality class. This has unanimously been corroborated by results obtained from various approaches [7], and has been commonly accepted.

Nevertheless, it is interesting to study these models in more detail, and in this short note we present results for periodic approximants for the Penrose and the Ammann-Beenker tiling. The zero-field Ising model on periodic approximants can be treated by methods that allow us to compute expansion coefficients and partition function zeros for the infinite periodic tiling, hence we do not have to deal with finite-size corrections as one usually accounts if only finite patches are considered. Instead, we can study the dependence on the size of the unit cell. From the partition function zeros, we obtain, in principle, the exact critical temperatures for the periodic approximants. In this way, we are able to derive precise estimates for the critical temperatures of the quasiperiodic models. For the high-temperature series of the free energy, we investigate the fluctuations in the sequence of expansion coefficients observed in [8], using the exact values for the critical temperatures of the periodic approximants.

2. The Ising model on periodic approximants

We place an “Ising spin” \( \sigma_i = \pm 1 \) on each vertex \( i \) of the periodic approximant. A configuration \( \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n) \) is assigned the energy

\[
E(\sigma) = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j
\]

(1)

where \( J > 0 \) is the ferromagnetic exchange coupling, which we choose identical for all pairs of neighbouring spins, and we sum over all neighbouring pairs of spins \( \langle i, j \rangle \) at vertices \( i \) and \( j \). Two vertices are neighbours if they are connected by an edge of the tiling.

There exist several variants for the solution of the zero-field Ising model; the method we use here was initially formulated by Kac and Ward for the square lattice Ising model [9]. The Kac-Ward determinant
and its application to periodic approximants was described in detail in our recent paper \[8\]. Let us just mention briefly that the partition function \( Z(\beta) = \sum_{\sigma} \exp[-\beta E(\sigma)] \) for a zero-field Ising model on an arbitrary planar graph, where \( \beta = 1/k_B T \) denotes the inverse temperature, is expressed as the square root of a determinant of an infinite matrix \( K(w) \), where \( w = \tanh(\beta J) \) \[10\]. For an infinite approximation, this matrix is cyclic. Thus the problem can, by Fourier transform, be reduced to the computation of a determinant of a finite matrix \( \tilde{K}(w, \varphi_1, \varphi_2) \) that depends on two additional parameters \( \varphi_1, \varphi_2 \in [0, 2\pi) \) which play the role of Bloch phases. The size of the matrix \( \tilde{K}(w, \varphi_1, \varphi_2) \) is given by the number of oriented edges in the unit cell, hence by \( 4N \) for the Penrose and the Ammann-Beenker approximants, where \( N \) denotes the number of spins in the unit cell. Apart from a factor \(-1/\beta\), the free energy per vertex in the thermodynamic limit \( f(w) = \lim_{M \to \infty} \log Z(\beta)/M \) is given as

\[
f(w) = \frac{1}{2N} \int_0^{2\pi} \int_0^{2\pi} \frac{d\varphi_1}{2\pi} \frac{d\varphi_2}{2\pi} \log \det \tilde{K}(w, \varphi_1, \varphi_2) \tag{2}\]

where \( M \) denotes the the number of spins in a finite patch approximating the infinite system.

For large approximants, it is expendable, and not very profitable, to compute the determinant analytically as a function of the parameters \( w, \varphi_1, \) and \( \varphi_2 \). Instead, we rather calculate the partition function zeros or the coefficients of the high-temperature expansion of the free energy by exploiting the fact that the matrix \( \tilde{K} \) has the form

\[
\tilde{K}(w, \varphi_1, \varphi_2) = I + w \tilde{L}(\varphi_1, \varphi_2) \tag{3}
\]

where \( I \) denotes the unit matrix. In particular, the matrix \( \tilde{L} \) does not depend on the variable \( w \). This makes it possible to compute the partition function zeros for given values of \( \varphi_1 \) and \( \varphi_2 \) from the eigenvalues of the matrix \( \tilde{L}(\varphi_1, \varphi_2) \), and the complete set of partition function zeros is just the accumulation of the zeros for all \( \varphi_1, \varphi_2 \in [0, 2\pi) \). The coefficients of the high-temperature expansion of the free energy

\[
f(w) = \sum_{n=2}^{\infty} g_{2n} w^{2n} \tag{4}\]

can be calculated from traces of powers of \( \tilde{L} \) by \[8\]

\[
g_{2n} = -\frac{1}{4nN} \int_0^{2\pi} \int_0^{2\pi} \frac{d\varphi_1}{2\pi} \frac{d\varphi_2}{2\pi} \text{tr}[\tilde{L}^{2n}(\varphi_1, \varphi_2)] \tag{5}\]

which follows by expanding the logarithm in Eq. (2).

3. Partition function zeros

In what follows, we adopt the usual convention and represent the partition function zeros in the variable \( z = (1+w)/(1-w) = \exp(2\beta J) \). For an infinite system, the zeros of the partition function in the complex \( z \) plane accumulate on lines or areas that separate different regions of analyticity of the free energy, hence different phases of the model. In particular, partition function zeros on the real axis correspond to phase transition points, and thus determine the critical temperature. The behaviour of zeros around these points is governed by the corresponding critical exponents \[11\].

From the present approach, it is obvious that the zeros themselves are parametrized by the two angles \( \varphi_1 \) and \( \varphi_2 \), thus we expect that they generically fill

![Fig. 1. Part of the partition function zeros in the complex \( z \) plane for the third periodic approximant of the Penrose tiling.](image1)

![Fig. 2. Same as Fig. 1 but for the second periodic approximant of the Ammann-Beenker tiling.](image2)
and the other for \(\phi\), two zeros on the positive real axis, one for \(\alpha\) further away from the positive real axis. We find the two circles found for the square lattice, in particular for the quasiperiodic case with an estimated error. Here, we show the zero patterns for the third approximant of the Ammann-Beenker tiling with \(N\) spins per unit cell. In Fig. 2. Here, the zeros were computed for angles \(\varphi_1, \varphi_2 \in \{m\pi/20 \mid m = 0, 1, 2, \ldots, 39\}\).

Clearly, the patterns are more complicated than the two circles found for the square lattice, in particular further away from the positive real axis. We find two zeros on the positive real axis, one for \(\varphi_1 = \varphi_2 = 0\) and the other for \(\varphi_1 = \varphi_2 = \pi\), corresponding to the ferromagnetic and antiferromagnetic critical points, respectively, which have the same properties due to the bipartiteness of the tilings. In the vicinity of the critical points, the zero patterns are very well described by segments of circles that orthogonally intersect the real axis, showing that the corresponding critical exponent \(\alpha\) stays the same as for the square lattice, i.e. \(\alpha = 0\), corresponding to a logarithmic singularity of the specific heat. The zeros on the real axis determine the critical temperatures for the periodic approximants, the results for the ferromagnetic critical point are shown in Tables 1 and 2. The values are in agreement with results of recent Monte Carlo simulations using the invaded cluster algorithm. Interestingly, the values for the Ammann-Beenker approximants in Table 2 appear to converge much faster than those for the Penrose case in Table 1.

This might be related to the observation that the mean coordination numbers, in particular the number of next-nearest neighbours, also converge faster for the Ammann-Beenker case, thus the periodic approximants of the Ammann-Beenker tiling are, in this sense, “closer” to the infinite quasiperiodic case than those of the Penrose tiling.

### 4. High-temperature expansion

In principle, the expansion coefficients of the high-temperature series can be calculated exactly for quasiperiodic cut-and-project tilings in the framework of the projection method. However, the number of graphs contributing to the expansion grows tremendously, thus limiting the applicability of this method. Recently, we presented the leading terms, up to 18th order in the expansion variable \(w = \tanh(\beta J)\), of the high-temperature series for the free energy \(f(w)\) of the Ising model on the Penrose and the Ammann-Beenker tiling. The series coefficients contain information about the critical behaviour of the model. Assuming that the free energy \(f(w)\) at the critical point \(w_c\) shows a power-law singularity \(f(w) \sim (1 - w^2/w_c^2)^{\kappa}\), the ratios of successive coefficients behave as

\[
\frac{g_{2n}}{g_{2n-2}} \sim \frac{1}{w_c^{\kappa}} \left(1 - \frac{\kappa + 1}{n}\right)
\]

for large \(n\), compare Eq. (4). Thus, plotting the ratio \(g_{2n}/g_{2n-2}\) as a function of \(1/n\), the data points should, for sufficiently large values of \(n\), lie on a straight line. From its intercept at \(1/n = 0\) and its slope, we can, in principle, extract the values of the critical temperature \(w_c\) and the critical exponent \(\kappa = 2 - \alpha = nd\). Here, \(d = 2\) denotes the spatial dimension, \(\nu\) is the critical exponent of the correlation length, which is \(\nu = 1\) for the Onsager universality class, and the last equality is due to scaling.

As shown in [4], this plot reveals large fluctuations, in particular for the smallest periodic approximants, while it behaves very nicely for simple lattices as, for instance, the square lattice. These fluctuations rendered impossible any reasonable estimate of the critical temperature or the critical exponent from the series expansion, at least in this way. In order to get

| \(m\) | \(N\) | \(w_c\) |
|---|---|---|
| 1 | 7 | 0.396 850 570 |
| 2 | 41 | 0.396 003 524 |
| 3 | 239 | 0.395 985 346 |
| 4 | 1393 | 0.395 984 811 |
| 5 | 8119 | 0.395 984 795 |
| \(\infty\) | \(\infty\) | 0.395 984 79(2) |

Table 1. Critical temperatures \(w_c = \tanh(J/k_B T_c)\) for periodic approximants of the Penrose tiling, extrapolated to the quasiperiodic case with an estimated error. Here, \(m\) labels the approximants with \(N\) spins per unit cell.
some more insight into the nature and the reasons of the fluctuations, we extended the series expansions for the periodic approximants considerably.

In Fig. 3, we plot the differences

\[ r_{2n} = \frac{n^3 - 3}{nw^2} \frac{g_{2n}}{g_{2n-2}} \]

between the ratios of the expansion coefficients, up to order \(2n = 128\), and their expected asymptotic behaviour for the three smallest periodic approximants of the Penrose tiling. Here, we use the critical temperatures \(w_c\) given in Table 1. Apparently, the ratios \(r_{2n}\) for the smallest approximant with \(N = 11\) spins per unit cell fluctuate strongly for \(20 \leq 2n \leq 60\). For larger values of \(2n\), the deviations from the asymptotic behaviour are small, similar to the square lattice case. The second approximant with \(N = 29\) shows a strikingly similar region with strong fluctuations, but at larger orders, starting around \(2n \geq 50\) and waning just around the maximal order \(2n = 128\) in Fig. 3. For the third approximant, no comparable region of particularly strong fluctuations is observed, but we might speculate that the order where these fluctuations occur grows roughly with the number of spins in the unit cell. In this case one has to go to higher orders to observe the effect. One might expect that for orders clearly beyond the number of oriented edges in the unit cell, i.e., for \(n \gg 4N\), the deviations from the asymptotic behaviour are small.

For larger approximants, the expansion coefficients \(g_{2n}\) rapidly approach those of the quasiperiodic tilings. Thus, we may draw the conclusion that the data for the periodic approximants show cross-over phenomena between the characteristic behaviour for the quasiperiodic model and the simple square-lattice case, although for the cases considered here the asymptotic behaviours should coincide. It seems reasonable that the cross-over occurs approxi-

mately at the size of the unit cell.

5. Concluding remarks

The Ising model defined on quasiperiodic tilings such as the Ammann-Beenker and the Penrose tiling belongs, according to scaling arguments, to the same universality class as the model on the square lattice. This is in accordance with our results on the partition function zeros and the high-temperature expansions for the corresponding periodic approximants. Nevertheless, the quasiperiodic systems show interesting features, and a better understanding of the cross-over phenomena in the high-temperature expansions of the periodic approximants is desirable.

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