Renormalization of two-dimensional Ising systems with irrelevant, marginal and relevant aperiodic (dis)order

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Abstract

We introduce a class of 2d Ising models with aperiodic modulations of the coupling constants following a 2d substitution rule. The relevance of the aperiodicity to the phase transition is examined through an approximative real space renormalization group (RG) approach known as the cumulant approximation. We find that the relevance of the aperiodic disorder is determined by the fluctuations of the mean coupling as predicted by the Harris-Luck criterion.

Keywords: quasicrystals, aperiodic order, renormalization group, Ising spin systems

1. Introduction

One important question in the study of aperiodic spin systems is how the introduction of the aperiodicity affects the critical properties of phase transitions. For Ising models, heuristic arguments led to the formulation of a relevance criterion [1], later called the Harris-Luck criterion, for rather general types of the aperiodicity (see Sec. 3 below). For a number of models with aperiodic modulations in one space direction, such as Ising quantum chains (or the equivalent 2d Ising model with layered aperiodicity), this criterion may even be derived exactly for any aperiodic order generated by substitution rules [2, 3].

Previous approaches to Ising models with 2d aperiodicity comprise exact [4, 5], approximate [6, 7], and numerical [8, 7] work (see [9] for further references). In general, they deal with specific quasiperiodic patterns, such as the Penrose tiling. In all these studies, universal critical behaviour of Onsager type was found, aperiodicity thus being *irrelevant*. In most cases, this agrees with the Harris-Luck criterion, which appeared to be rather well confirmed also in 2d that way. However, one of the few exact results is a notable exception, even if the aperiodicity involved is too special to give a real check for the generic case: In the solvable class of the so-called labyrinth models aperiodicity is always irrelevant [9], even if, in some cases, the Harris-Luck criterion predicts otherwise.

In the following, we present a RG study for a large class of models with irrelevant, marginal and relevant aperiodic order. While previous results all deal with irrelevant aperiodicity, this should provide a profound check for the Harris-Luck criterion in 2d.

2. 2d substitutions on the square lattice

We define a 2d substitution rule ϱ on an alphabet $\mathcal{A} = \{a_1, \ldots, a_n\}$ of n letters by the following scheme:

$$\varrho : a_i \mapsto \begin{matrix} w_i^2 & w_i^3 \\ w_i^1 & w_i^2 \end{matrix} \; ; \quad w_i^j \in \mathcal{A} \; . \tag{1}$$

Patterns generated that way may describe an aperiodic distribution of n different sorts of atoms on a square lattice. While this kind of *chemical* disorder is known from incommensurable phases [10], *topological* disorder, as met in 2d quasicrystals, is not included in this scheme. Nevertheless, the structures show many typical properties of aperiodic long range order, making them an interesting object for theoretical studies. Although this has been suggested already in [11] (for 2d tight binding models) no such study, to our knowledge, has been published so far.

Note that one entry, w_i^2, appears twice in the substitution scheme (1). This guarantees the equivalence of the aperiodicity in both space directions. An extension to the general case is no problem in principle but leads to somewhat clumsier formulas.

3. Fluctuations and the Harris-Luck criterion

Using heuristic scaling arguments, the following criterion for the relevance of aperiodic disorder in ferromagnetic Ising systems with correlation length exponent ν_0 in the unperturbed case has been given in [1]: Aperiodic modulations in d_m dimensions are relevant iff the fluctuation exponent ω of the mean coupling strength exceeds a critical value ω_c:

$$\omega > \omega_c = 1 - \frac{1}{d_m \nu_0} \ . \tag{2}$$

This is the so-called *Harris-Luck criterion.* With the Onsager value $\nu_0 = 1$ it predicts $\omega_c = 1/2$ for the 2d Ising model with isotropic aperiodicity.

If the ordering of the coupling constants is directly given by a substitution rule, the fluctuation exponent may be determined from the leading and next-to-leading eigenvalues $\lambda_{1,2}$ of the corresponding substitution matrix [1, 3] as: $\omega = 0$ for $|\lambda_2| \le 1$ and

$$\omega = \frac{\log|\lambda_2|}{\log \lambda_1} \quad \text{for} \quad |\lambda_2| > 1 \ . \tag{3}$$

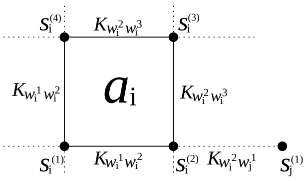
4. Model and block spin transformation

Consider the Hamiltonian of the 2d Ising model,

$$H(\boldsymbol{s}) = \sum_{<k,k'>} K(k,k')s(k)s(k') \ ; \quad s(k) = \pm 1 \tag{4}$$

where the Boltzmann factor $\beta = 1/k_B T$ is included in the nearest neighbour interactions $K(k,k')$. The strength of the couplings shall vary aperiodically according to the substitution scheme defined in (1). This is done by dividing the square lattice in blocks of 4 spins each and defining a local parametrization of the spins and couplings in the following way

$$\varrho(a_i) = \begin{matrix} w_i^2 & w_i^3 \\ w_i^1 & w_i^2 \end{matrix} \quad \curvearrowright$$



Spins carry indices for the block and the position within the block, couplings are labeled via their endpoints according to the substitution rule ϱ. Note that, since the action of ϱ on the couplings is *indirect* here, some care has to be taken in the application of formula (3) for the fluctuation exponent (see below).

The basic plan for the renormalization follows the obvious idea to invert the substitution process. In every RG step, the Hamiltonian H shall be mapped to a renormalized Hamiltonian $\tilde{H}$ with coupling constants $\tilde{K}$ that describe the effective interaction between adjacent 4-spin-blocks. However, in contrast to the 1d case, the iterated summation of spin degrees of freedom in 2d finite blocks inevitablely generates spin interactions of increasing range as well as multi-spin couplings. Since an exact formulation of the RG including all sorts of couplings seems impossible, we have to rely on approximative methods. There are different possibilities. The simplest methods, like the *Migdal-Kadanoff* scheme, use a naive decimation of part of the spin degrees of freedom (3 out of 4 in each block in our case). For quasiperiodic models, this scheme has been used for Ising models on Penrose tilings [12] and 2d Fibonacci grids [13]. However, with this method, even the results for periodic models differ quite substantially from the exact values. A study of the relevance of aperiodic disorder in the above class of models does not lead to a clear picture. Other methods try to sum over degrees of freedom with higher energies. One way to do this is the so-called *block spin transformation.* Here, the direction of the renormalized *block spin*, $\tilde{s}$, is given by the majority of the spins in the block and assumes either value $\tilde{s} = \pm 1$ with equal probability in the case of a tie. This way, a weight function $P(\tilde{\boldsymbol{s}}, \boldsymbol{s})$ is defined that determines the transition probability for any configuration of block spins $\tilde{\boldsymbol{s}}$, given the configuration of spins $\boldsymbol{s}$ in the original Hamiltonian.

5. The cumulant approximation

The cumulant approximation is a block spin transformation for 2d Ising models. Originally, the method has been introduced for the triangular lattice [14, 15], but can be applied to quite a variety of lattices and graphs. In the context of aperiodic disorder, the method has been used for models on the duals of the Penrose [6] and Ammann-Beenker tilings [7]. In both cases, aperiodic disorder is irrelevant, in accordance with the Harris-Luck criterion. While for a detailed discussion we refer to [15], the main idea of the cumulant approximation is as follows: The original Hamiltonian is split into two parts, $H = H_0 + V$, H_0 describing the couplings within the spin blocks and V the interactions in between the blocks. To leading order, the block interaction V is then approximated by its expectation value with respect to H_0,

$$\langle V \rangle(\tilde{s}) = \frac{\sum_{\{\boldsymbol{s}\}} P(\tilde{\boldsymbol{s}}, \boldsymbol{s}) V(\boldsymbol{s}) \exp[H_0(\boldsymbol{s})]}{\sum_{\{\boldsymbol{s}\}} P(\tilde{\boldsymbol{s}}, \boldsymbol{s}) \exp[H_0(\boldsymbol{s})]} \ . \tag{5}$$

Higher order corrections my be given as a formal expansion in the cumulants $(V - \langle V \rangle)^k$ [15]. However, since these terms do not add any further insight into our qualitative results, we will not include them in this short exposition.

Since V contains all interactions between the blocks, we may now use (5) to obtain an effective block spin interaction. Using the parametrization of the couplings and spins defined above, we obtain the following RG equations:

$$\tilde{K}_{a_i a_j} = K_{w_i^2 w_j^1} \langle s_i^{(2)} \rangle \langle s_j^{(1)} \rangle + K_{w_i^3 w_j^2} \langle s_i^{(3)} \rangle \langle s_j^{(2)} \rangle . \quad (6)$$

The fixed point of this transformation is $K_{a_i a_j} \equiv K_0$,

$$K_0 = \frac{1}{4} \log \left[1 + 2\sqrt{2} + \sqrt{5(2+\sqrt{2})} \right] . \quad (7)$$

For an arbitrary substitution rule, the entries of the Jacobian $\boldsymbol{dK}$ at the fixed point are

$$\begin{aligned} \frac{\partial \tilde{K}_{a_i a_j}}{\partial K_{a_k a_\ell}} \Big|_{K_0} &= \frac{1}{2} \left(\delta_{w_i^2, a_k} \delta_{w_j^1, a_\ell} + \delta_{w_i^3, a_k} \delta_{w_j^2, a_\ell} \right) \\ &+ \left(\delta_{w_i^1, a_k} \delta_{w_i^2, a_\ell} + \delta_{w_j^2, a_k} \delta_{w_j^3, a_\ell} \right) E_- \\ &+ \left(\delta_{w_i^2, a_k} \delta_{w_i^3, a_\ell} + \delta_{w_j^1, a_k} \delta_{w_j^2, a_\ell} \right) E_+ \quad (8) \end{aligned}$$

where

$$E_+ = \frac{2K_0}{7} \left(10 - 11\sqrt{2} + e^{4K_0} \right) \simeq 0.35618 \quad (9)$$

$$E_- = \frac{2K_0}{7} \left(2 - 11\sqrt{2} + (2\sqrt{2}-1) e^{4K_0} \right) \simeq 0.14791 \quad (10)$$

As usual, spectrum and eigenbasis of $\boldsymbol{dK}$ determine the renormalization flow in the vicinity of the fixed point. The leading eigenvalue of $\boldsymbol{dK}$ turns out to be independent of the substitution rule,

$$\lambda_T = 1 + 2(E_+ + E_-) \simeq 2.0081761785 . \quad (11)$$

It corresponds to the scaling field of the reduced temperature and we obtain as the corresponding RG eigenvalue within the cumulant approximation

$$y_T = \frac{\log \lambda_T}{\log 2} \simeq 1.0058858433 , \quad (12)$$

which should be compared with the exact Onsager value $y_T = 1$. As long as y_T is the only relevant eigenvalue (as for uniform couplings), the model remains in the Onsager universality class with scaling exponents $\alpha = 2 - 2/y_T$ and $\nu = 1/y_T$. We expect aperiodic disorder to alter the critical scaling iff there is at least one further RG eigenvalue outside the unit circle. In the following, we show how that may be seen from the spectrum of the substitution matrix.

6. Substitution and renormalization

The RG transformation is a mapping in the space of the coupling constants. In order to relate this mapping to the substitution process that is originally defined on the spins, we now consider the induced action of the substitution process on the couplings. We introduce a *bond substitution rule* $\hat{\varrho}$ on pairs of adjacent letters (which label the couplings) as follows:

$$\hat{\varrho} : \; a_i \text{---} a_j \;\longmapsto\; \begin{array}{c} w_i^2 \overset{c}{\text{---}} w_i^3 \overset{1}{\text{---}} w_j^2 \overset{1-c}{\text{---}} w_j^3 \\ \\ w_i^1 \overset{c'}{\text{---}} w_i^2 \overset{1}{\text{---}} w_j^1 \overset{1-c'}{\text{---}} w_j^2 \end{array} . \quad (13)$$

For couplings within columns, we obtain a mirror reflected and 90^o rotated scheme. The numbers above the couplings on the right hand side of (13) are weight factors. For a consistent substitution, c and c' may assume any value in the interval $[0,1]$. The substitution matrix of $\hat{\varrho}$ has the following entries

$$\begin{aligned} [M_{\hat{\varrho}}]_{ij,k\ell}(c,c') = \#_{a_k a_\ell}[\hat{\varrho}(a_i a_j)] = \delta_{w_i^2, a_k} \delta_{w_j^1, a_\ell} + \\ \delta_{w_i^3, a_k} \delta_{w_j^2, a_\ell} + c \cdot \delta_{w_i^2, a_k} \delta_{w_i^3, a_\ell} + (1-c) \cdot \delta_{w_i^1, a_k} \delta_{w_i^2, a_\ell} \\ + c' \cdot \delta_{w_j^2, a_k} \delta_{w_j^3, a_\ell} + (1-c') \cdot \delta_{w_j^1, a_k} \delta_{w_j^2, a_\ell} . \quad (14) \end{aligned}$$

Comparing $\boldsymbol{M}_{\hat{\varrho}}(c,c')$ with the Jacobian $\boldsymbol{dK}$ of the RG (8) we find, up to a small error δ:

$$\boldsymbol{dK} \simeq \frac{1}{2} \boldsymbol{M}_{\hat{\varrho}}^t (2E_+, 1 - 2E_+) := \frac{1}{2} \boldsymbol{M}_{\hat{\varrho}}^t [E_+] . \quad (15)$$

The error may be expressed as a shift of E_-,

$$E_- \longrightarrow E_- - \delta \equiv 0.5 - E_+ \; ; \quad \delta \simeq 0.004088 . \quad (16)$$

Up to the same small error that already appeared in the approximation of the temperature eigenvalue y_T, the Jacobian of the cumulant expansion coincides with half of the transposed substitution matrix of $\hat{\varrho}$. Within the approximation, we may thus replace the RG matrix $\boldsymbol{dK}$ by $\frac{1}{2}\boldsymbol{M}_{\hat{\varrho}}^t[E_+]$, thereby shifting the temperature eigenvalue to the correct value $y_T = 1$. Now, aperiodic modulations should be relevant iff λ_2, the second largest eigenvalue of $\boldsymbol{M}_{\hat{\varrho}}[E_+]$, is larger than 2 in absolute value. However, since the substitution $\hat{\varrho}$ acts directly on the coupling constants, we may now use (3) to rewrite this as a condition for the fluctuation exponent ω. In the class of models introduced above, aperiodic disorder is relevant iff

$$\omega = \frac{\log |\lambda_2|}{\log 4} > \omega_c = \frac{1}{2} . \quad (17)$$

Fluctuations thus have to be stronger than in the uncorrelated case where $\omega = 1/2$. This, however, is just the prediction of the Harris-Luck criterion (2).

We have related the RG matrix $\boldsymbol{dK}$ to the substitution matrix $\boldsymbol{M}_{\hat{\varrho}}(c,c')$ at a special value of c and c'. But in fact, as is easily shown, no eigenvalue $|\lambda| \geq 2$ of $\boldsymbol{M}_{\hat{\varrho}}$ depends on c or c'. The fluctuation exponent ω and the relevance of the aperiodicity are therefore independent of the exact setup of the bond substitution $\hat{\varrho}$, as it should be. Furthermore, the most important information is already contained in the spectrum of the original spin substitution ϱ: the spectrum of the bond substitution matrix $\boldsymbol{M}_{\hat{\varrho}}(c,c')$ contains the spectrum of the spin substitution ϱ for arbitrary c,c', and all additional eigenvalues are $|\lambda| \leq 2$. We thus find that aperiodic disorder is *relevant* iff the second largest eigenvalue of the substitution matrix of the spin substitution ϱ is $|\lambda_2| > 2$.

7. Examples

(I) The substitution rule

$$\varrho: \; a \mapsto \begin{matrix} b & a \\ a & b \end{matrix} \; ; \quad b \mapsto \begin{matrix} a & b \\ b & a \end{matrix} \tag{18}$$

defines a pattern with a *Thue-Morse sequence* in every row and column. The pattern has the full D_4 symmetry of the square lattice. We find as second largest eigenvalue $\lambda_2 = -2$ (*exactly*, also for the original RG matrix $\boldsymbol{dK}$), indicating *marginal* aperiodicity. One shows that the marginal scaling field just vanishes at the *self-dual point* of the model, $K_{aa} = K_{ab}$; $K_{ba} = K_{bb}$, leading to universal scaling.

(II) The substitution rule

$$\varrho: \; \begin{matrix} a \mapsto \begin{matrix} b & a \\ a & b \end{matrix} \; ; \quad b \mapsto \begin{matrix} a & c \\ c & a \end{matrix} \\ \\ c \mapsto \begin{matrix} d & b \\ b & d \end{matrix} \; ; \quad d \mapsto \begin{matrix} c & d \\ d & c \end{matrix} \end{matrix} \tag{19}$$

generates a kind of 2d counterpart of the 1d *Rudin-Shapiro* chain. The pattern has D_4 symmetry if the lattice is labelled with a binary code according to $a,b \to 1$ and $c,d \to 0$. In this case, the second largest eigenvalue is $\lambda_2 = \pm 2\sqrt{2}$ ($\lambda_2 \approx \pm 2.8240$ in the original RG matrix $\boldsymbol{dK}$). We thus find $\omega = 3/4$ and fluctuations are stronger than for randomly distributed couplings. Aperiodicity is *relevant* and we expect a changed critical scaling behaviour.

8. Discussion

We introduced a class of 2d Ising models with 2d aperiodic modulations of the coupling constants. Within a well-known approximative real space RG scheme, the heuristic Harris-Luck relevance criterion has been confirmed for these models. Similar to the case of 1d aperiodicity [2], the substitution matrix of the substitution that generates the underlying aperiodic order determines (up to a small shift) the RG eigenvalues and scaling fields of the model. The extra factor of 2 in comparison with the 1d case accounts for the dimension parameter in the Harris-Luck formula.

Certainly, no exact derivation of a relevance criterion can be obtained by an approximative method. But at least, our result shows a non-trivial consistency and also indicates that the cumulant approximation is indeed a suitable tool for the study of aperiodic structures, leading to reasonable results.

Besides these qualitative results, the significance of the cumulant approximation as a quantitative method is certainly limited. The surprisingly precise prediction of the exponents ν and α for models with irrelevant aperiodicity (deviation from the exact Onsager values less than 0.6%) must be seen relative to the fact that the error is up to an order of magnitude higher for other lattices (such as the triangular lattice or the Penrose graph). More importantly, the method does not provide any information on the changed scaling behaviour in the marginal or relevant case. Certainly one should expect the critical singularities to be weakened (as it is the case for 1d aperiodicity). A detailed study, however, remains to be done. For the class of models introduced here, this should be possible numerically, at least in the case of relevant aperiodic disorder.

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