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Surface magnetization of aperiodic Ising systems: a comparative study of the bond and site problems

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Abstract. We investigate the influence of aperiodic perturbations on the critical behaviour at a second-order phase transition. The bond and site problems are compared for layered systems and aperiodic sequences generated through substitution. In the bond problem, the interactions between the layers are distributed according to an aperiodic sequence whereas in the site problem, the layers themselves follow the sequence. A relevance–irrelevance criterion introduced by Luck for the bond problem is extended to discuss the site problem. It involves a wandering exponent for pairs, which can be larger than the one considered previously in the bond problem. The surface magnetization of the layered two-dimensional Ising model is obtained, in the extreme anisotropic limit, for the period-doubling and Thue–Morse sequences.

1. Introduction

The discovery of quasicrystals (Schechtman *et al* 1984) has opened a new field of research which has been quite active during the last ten years (see Henley 1987, Janssen 1988, Janot *et al* 1989, Guyot *et al* 1991, Steinhardt and DiVicenzo 1991). On the theoretical side, quasiperiodic or, more generally, aperiodic systems are interesting because they appear as intermediates between periodic and random systems. Thus, phase transitions in such systems are expected to display a rich and unusual critical behaviour.

Studies of the Ising model (Godreche *et al* 1986, Okabe and Niizeki 1988, Sørensen *et al* 1991), the percolation problem (Sakamoto *et al* 1989, Zhang and De'Bell 1993) and the statistics of self-avoiding walks (Langie and Iglói 1992) on the two-dimensional Penrose lattice did not show any change of critical exponents. Universal behaviour was also obtained in three dimensions (Okabe and Niizeki 1990). But some systems were also found for which the aperiodicity has some influence. One may mention interface roughening in two dimensions for which a continuously varying roughness exponent was obtained with the Fibonacci sequence (Henley and Lipowsky 1987, Garg and Levine 1987).

Some exact results have been obtained for the layered Ising model with an aperiodic modulation of the interlayer couplings (Iglói 1988, Doria and Satija 1988, Benza 1989, Henkel and Patkós 1992, Lin and Tao 1992, Turban and Berche 1993). The problem was studied in the extreme anisotropic limit where it leads to a one-dimensional aperiodic quantum Ising model (QIM) in a transverse field, which is often easier to handle (Kogut 1979). For the Fibonacci and other sequences, the specific heat was found to display the Onsager logarithmic singularity but for different sequences the singularity is washed out

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(Tracy 1988), like in the randomly layered Ising model (McCoy and Wu 1968a, 1968b, McCoy 1970).

The situation was clarified in a recent study of the bulk properties of the QIM (Luck 1993a). In this work, Luck proposed a generalization for aperiodic systems of the Harris criterion (Harris 1974), allowing a classification of critical aperiodic systems according to the sign of a crossover exponent Φ . This exponent involves the correlation length exponent of the unperturbed system ν and the wandering exponent ω governing the size-dependence of the fluctuations of the aperiodic interactions (Dumont 1990). The criterion has also been applied to the case of anisotropic critical systems with uniaxial aperiodicity (Iglói 1993), explaining the interface roughening results. It was later generalized to d -dimensional aperiodicities in isotropic critical systems (Luck 1993b). The form of the singularities with a relevant aperiodic perturbation has been discussed by Iglói using scaling arguments (Iglói 1993). Recently, some exact results for the surface magnetization of the QIM have also been obtained for irrelevant, marginal and relevant aperiodicities (Turban *et al* 1994, Iglói and Turban 1994) and conformal aspects have been discussed (Grimm and Baake 1994).

Most of the systems treated so far dealt with an aperiodic distribution of the couplings, i.e. with the *bond problem*. In magnetic systems, this corresponds to an aperiodic distribution of the atoms mediating the interactions in a superexchange mechanism. In the present work, we study the surface magnetization of the aperiodic QIM, comparing the bond problem examined previously (Turban *et al* 1994, Iglói and Turban 1994) to the *site problem* for which the magnetic moments are distributed aperiodically and interact through a direct exchange mechanism. Then the couplings depend on the nature of the two atoms involved in the interaction. We show that, for a given aperiodic sequence, the perturbation may be more efficient for the site than for the bond problem and may lead to a different critical behaviour. Exact results are obtained for two typical aperiodic sequences.

In section 2 we present the Hamiltonian of the QIM and give the expression of the surface magnetization, defining the parameters for the bond and site problems. In section 3 we recall the properties of the substitution matrix, associated with an aperiodic sequence generated through an inflation rule, for the bond problem. The substitution matrix adapted to the site problem is defined and compared to the previous one in section 4. Then the relevance-irrelevance criterion is discussed (section 5) and some general results about the QIM critical coupling and surface magnetization are presented (section 6). The period-doubling and Thue-Morse sequences are studied in sections 7 and 8 and the final section contains a summary and discussion.

2. Hamiltonian and surface magnetization

Let us consider a layered semi-infinite two-dimensional Ising model with exchange interactions $K_1(k)$ parallel to the surface and $K_2(k)$ between the layers at k and $k+1$ (in $k_B T$ units). The extreme anisotropic limit (Kogut 1979) corresponds to $K_1(k) \rightarrow \infty$, $K_2(k) \rightarrow 0$ while keeping the ratio $\lambda_k = K_2(k)/K_1^*(k)$ fixed. In this expression $K_1^*(k) = -\frac{1}{2} \ln \tanh K_1(k)$ is a dual coupling which goes to zero in the limit. Introducing a constant reference coupling K_1^* , the dual coupling can be rewritten as $h_k K_1^*$, where h_k is the transverse field. The transfer operator $\exp(-2K_1^* \mathcal{H})$ involves the Hamiltonian of a one-dimensional spin- $\frac{1}{2}$ quantum chain. Introducing the two-spin interactions $J_k = h_k \lambda_k$, the QIM takes the following form:

$$\mathcal{H} = -\frac{1}{2} \sum_{k=1}^{\infty} [h_k \sigma_k^z + J_k \sigma_k^x \sigma_{k+1}^x] \quad (2.1)$$

where the σ 's are Pauli spin operators.

The Hamiltonian can be put in diagonal form (Lieb *et al* 1961)

$$\mathcal{H} = \sum_{\nu} \epsilon_{\nu} (\eta_{\nu}^{\dagger} \eta_{\nu} - \frac{1}{2}) \quad (2.2)$$

using the Jordan–Wigner transformation (Jordan and Wigner 1928) followed by a canonical transformation to the diagonal fermion operators η_{ν} . The fermion excitation spectrum is obtained as the solution of the eigenvalue problem

$$\begin{aligned} \epsilon_{\alpha} \psi_{\alpha}(k) &= -h_k \phi_{\alpha}(k) - J_k \phi_{\alpha}(k+1) \\ \epsilon_{\alpha} \phi_{\alpha}(k) &= -J_{k-1} \psi_{\alpha}(k-1) - h_k \psi_{\alpha}(k) \\ h_0 &= J_0 = 0 \end{aligned} \quad (2.3)$$

where the $\phi_{\alpha}(k)$ and $\psi_{\alpha}(k)$ are the components of two normalized eigenvectors which satisfy the boundary conditions $\phi_{\alpha}(0) = \psi_{\alpha}(0) = 0$.

In the ordered phase, the two-spin correlation function in the surface asymptotically gives the square of the surface magnetization, which can be written as the matrix element $m_s = \langle 1 | \sigma_1^x | 0 \rangle$ between the ground state and the first excited state of the Hamiltonian. For the semi-infinite system these two states become degenerate in the ordered phase, i.e. the lowest excitation ϵ_1 vanishes. Using the above-mentioned transformation to diagonal fermions, it can be shown that m_s is also given by $\phi_1(1)$. According to the first equation in (2.3) with $\epsilon_{\alpha} = 0$, the other components of the eigenvector can be deduced from the recursion relation

$$\phi_1(k+1) = -\frac{h_k}{J_k} \phi_1(k) = -\lambda_k^{-1} \phi_1(k). \quad (2.4)$$

The normalization of the eigenvector then leads to the surface magnetization (Peschel 1984)

$$m_s = \left(1 + \sum_{j=1}^{\infty} \prod_{k=1}^j \lambda_k^{-2} \right)^{-1/2} \quad (2.5)$$

where the couplings J_k and h_k in \mathcal{H} only enter through their ratio λ_k . Thus m_s is the same as for a quantum chain with $h_k = 1$ and an effective two-spin interaction λ_k . Such a reparametrization of the Hamiltonian is no longer possible when non-vanishing excitations are involved, if the transverse field is k -dependent. It follows that, in general, the effect of both interactions have to be considered. We shall come back to this point in section 5.

In the bond problem the interactions parallel to the surface are constant, $K_1(k) = K_1$, so that $h_k = 1$ and $\lambda_k = K_2(k)/K_1^*$ depends on the layer index k only through the value of the interlayer interaction. In the site problem, the effective coupling $\lambda_k = K_2(k)/K_1^*(k)$ involves both the interaction inside layer k and the interaction between layers k and $k+1$. As a consequence, its value depends on the nature of the two layers and it is generally asymmetric.

3. Substitution matrix for the bond problem

In this section we give a brief summary of the properties of aperiodic sequences generated through an inflation rule. To simplify the presentation, we consider sequences involving

only two letters, A and B. In the bond problem these letters correspond to the interlayer interactions λ_A, λ_B . The generalization to any number of letters is straightforward.

A sequence is constructed through iterated substitutions on the two letters, $A \rightarrow S\{A\}$, $B \rightarrow S\{B\}$. The process will be illustrated on the following example:

$$\begin{aligned} S\{A\} &= B A A \\ S\{B\} &= A B . \end{aligned} \quad (3.1)$$

When the construction starts on A, after n steps, one obtains

$$\begin{aligned} n = 0 & \quad A \\ n = 1 & \quad B A A \\ n = 2 & \quad A B B A A B A A \\ & \quad \vdots \end{aligned} \quad (3.2)$$

whereas, starting on B, the iteration gives

$$\begin{aligned} n = 0 & \quad B \\ n = 1 & \quad A B \\ n = 2 & \quad B A A A B \\ & \quad \vdots \end{aligned} \quad (3.3)$$

Information about the sequence is contained in the substitution matrix

$$\mathbf{M}_1 = \begin{pmatrix} n_A^{S\{A\}} & n_A^{S\{B\}} \\ n_B^{S\{A\}} & n_B^{S\{B\}} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \quad (3.4)$$

where the matrix elements give the numbers of A or B in $S\{A\}$ or $S\{B\}$. It is easy to check that the numbers L_n^A and L_n^B of A and B in the sequence, after n substitutions, are given by the corresponding matrix elements in \mathbf{M}_1^n . They belong to the first (second) column when the construction starts on A (B).

Let V_α be the right eigenvectors and Λ_α the eigenvalues of the substitution matrix such that

$$\mathbf{M}_1 V_\alpha = \Lambda_\alpha V_\alpha . \quad (3.5)$$

L_n^A, L_n^B and the length of the sequence, L_n , are asymptotically proportional to Λ_1^n where $\Lambda_1 > 1$ is the eigenvalue of \mathbf{M}_1 with largest modulus, which is real and positive according to the Perron-Frobenius theorem. The asymptotic density, $\rho_\infty^A = \lim_{n \rightarrow \infty} L_n^A / L_n$, can be deduced from the associated eigenvector with

$$\rho_\infty^A = 1 - \rho_\infty^B = \frac{V_1(1)}{V_1(1) + V_1(2)} . \quad (3.6)$$

The interactions in the bond problem can be rewritten as

$$\lambda_A = \bar{\lambda} + \rho_\infty^B \delta_1 \quad \lambda_B = \bar{\lambda} - \rho_\infty^A \delta_1 \quad (3.7)$$

where $\bar{\lambda}$ is the averaged coupling and $\delta_1 = \lambda_B - \lambda_A$, the amplitude of the aperiodic modulation. At a length scale L_n , the cumulated deviation from the average is

$$\Delta_1(L_n) = \sum_{k=1}^{L_n} (\lambda_k - \bar{\lambda}) \sim \delta_1 \Lambda_2^n \sim \delta_1 L_n^{\omega_1} \tag{3.8}$$

where Λ_2 is the second largest eigenvalue in modulus. The wandering exponent

$$\omega_1 = \frac{\ln |\Lambda_2|}{\ln \Lambda_1} \tag{3.9}$$

governs the behaviour of the fluctuations of the interlayer couplings (Dumont 1990).

4. Substitution matrix for the site problem

Let us now consider the site problem. The two letters A and B then correspond to the two magnetic species which are distributed according to the aperiodic sequence, with the layers containing either A or B atoms. The QIM effective couplings λ_{AA} , λ_{AB} , λ_{BA} and λ_{BB} depend on the nature of the two layers involved in the interaction through the intra- and interlayer couplings in the anisotropic classical system.

In order to count the numbers of bonds of different types in the sequence after n substitutions, L_n^{AA} , L_n^{AB} , L_n^{BA} and L_n^{BB} , one defines the two-letter substitution matrix

$$\mathbf{M}_2 = \begin{pmatrix} n_{AA}^{S\{A\{A\}} & n_{AA}^{S\{A\{B\}} & n_{AA}^{S\{B\{A\}} & n_{AA}^{S\{B\{B\}} \\ n_{AB}^{S\{A\{A\}} & n_{AB}^{S\{A\{B\}} & n_{AB}^{S\{B\{A\}} & n_{AB}^{S\{B\{B\}} \\ n_{BA}^{S\{A\{A\}} & n_{BA}^{S\{A\{B\}} & n_{BA}^{S\{B\{A\}} & n_{BA}^{S\{B\{B\}} \\ n_{BB}^{S\{A\{A\}} & n_{BB}^{S\{A\{B\}} & n_{BB}^{S\{B\{A\}} & n_{BB}^{S\{B\{B\}} \end{pmatrix} = \begin{pmatrix} 1 & 2 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{4.1}$$

where, for example, $n_{AB}^{S\{B\{A\}}$ gives the number of AB-bonds in the sequence generated by $S\{B\}$ complemented by the first letter in $S\{A\}$. Such a sequence builds the first part of the sequence which is obtained when the inflation rule is applied to a BA-bond. The same matrix \mathbf{M}_2 has been considered before as resulting from substitutions on words of length two (Queffelec 1987).

With the example of the previous section, the two-letter substitutions read

$$\begin{aligned} S\{A\{A\} &= B A A [B] \\ S\{A\{B\} &= B A A [A] \\ S\{B\{A\} &= A B [B] \\ S\{B\{B\} &= A B [A] \end{aligned} \tag{4.2}$$

and lead to the last matrix in (4.1).

As before, the matrix elements in each column of \mathbf{M}_2^n give the numbers of bonds of each type (L_n^{ij} ; $i, j = A, B$) in the sequence obtained after n iterations. These numbers are found in the two first (last) columns if the construction starts on A (B) and are given by the minimum of the two values appearing in each half-row. Due to end effects, one of

the values in each column differs by 1 from the true number of bonds in the sequence. At $n = 2$, for example, we have

$$\mathbf{M}_2^2 = \begin{pmatrix} 3 & 2 & 2 & 2 \\ 2 & 3 & 1 & 1 \\ 2 & 2 & 2 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix}. \tag{4.3}$$

The first two columns correspond to a sequence constructed on A at the second iteration and lead to $L_2^{AA}=2, L_2^{AB}=2, L_2^{BA}=2$ and $L_2^{BB}=1$, in agreement with (3.2).

Since the sum of the numbers of bonds starting with a given letter (i.e. with A, AA and AB bonds) gives the number of times this letter is met in the sequence for the bond problem, the matrix elements of \mathbf{M}_1 are recovered by taking the sum of the two first elements and the sum of the two last elements in each column of \mathbf{M}_2 . The same results are obtained with the two first (last) columns since the corresponding sequences only differ through their last bond. The same relation exists between the elements of \mathbf{M}_2^n and \mathbf{M}_1^n .

Let Ω_α be the eigenvalues and \mathbf{W}_α the right eigenvectors of \mathbf{M}_2 . The numbers of bonds L_n^{ij} ($i, j = A, B$) in the sequence after n iterations are still proportional to the n th power of the largest eigenvalue Ω_1 . Using the associated eigenvector, one obtains the asymptotic bond densities

$$\begin{aligned} \rho_\infty^{AA} &= \frac{W_1(1)}{\sum_{i=1}^4 W_1(i)} & \rho_\infty^{AB} &= \frac{W_1(2)}{\sum_{i=1}^4 W_1(i)} \\ \rho_\infty^{BA} &= \frac{W_1(3)}{\sum_{i=1}^4 W_1(i)} & \rho_\infty^{BB} &= \frac{W_1(4)}{\sum_{i=1}^4 W_1(i)}. \end{aligned} \tag{4.4}$$

Since the length of the sequence after n steps is also the sum of the L_n^{ij} , the leading eigenvalues of the two matrices are the same. Using the above-mentioned relation between the matrix elements of \mathbf{M}_2 and \mathbf{M}_1 , the secular equation of \mathbf{M}_2 can be factorized. The first factor gives back the secular equation of \mathbf{M}_1 so that $\Omega_1 = \Lambda_1$ and Λ_2 also belongs to the spectrum of \mathbf{M}_2 . The two last eigenvalues of \mathbf{M}_2 follow from the second factor and read

$$\Omega_\alpha = \frac{1}{2} [a + b \pm \sqrt{(a - b)^2 + 4cd}] \tag{4.5}$$

where

$$\begin{aligned} a &= n_{AA}^{S\{A\{A\}} - n_{AA}^{S\{A\{B\}} & b &= n_{BA}^{S\{B\{A\}} - n_{BA}^{S\{B\{B\}} \\ c &= n_{BA}^{S\{A\{A\}} - n_{BA}^{S\{A\{B\}} & d &= n_{AA}^{S\{B\{A\}} - n_{AA}^{S\{B\{B\}}. \end{aligned} \tag{4.6}$$

Since the coefficients in (4.6) involve differences between the numbers of bonds in sequences which at most differ through their last bond, they are equal to 0 or ± 1 . They are completely determined through the first and last letters in $S\{A\}$ and $S\{B\}$ and can be obtained by inspection. The two eigenvalues are also equal to 0 or ± 1 . When the two substitutions begin with the same letter, the coefficients and the eigenvalues Ω_α vanish. Other cases are listed in table 1.

As in the bond problem, the fluctuations in the couplings λ_k can be deduced from the substitution matrix, working in the basis of the right eigenvectors \mathbf{W}_α . The averaged coupling $\bar{\lambda}$ is now given by

$$\bar{\lambda} = \rho_\infty^{AA} \lambda_{AA} + \rho_\infty^{AB} \lambda_{AB} + \rho_\infty^{BA} \lambda_{BA} + \rho_\infty^{BB} \lambda_{BB}. \tag{4.7}$$

Table 1. Coefficients of the secular equation (4.5) and corresponding eigenvalues for substitutions starting with different letters.

$S\{A\}$	A...A	A...A	A...B	A...B	B...A	B...A	B...B	B...B
$S\{B\}$	B...A	B...B	B...A	B...B	A...A	A...B	A...A	A...B
a	1	1	0	0	-1	-1	0	0
b	0	1	0	1	0	-1	0	-1
c	1	0	1	0	-1	0	-1	0
d	0	0	1	1	0	0	-1	-1
Ω_z	1, 0	1, 1	1, -1	1, 0	-1, 0	-1, -1	1, -1	-1, 0

The cumulated deviation from $\bar{\lambda}$ is generally governed by Ω_2 , the second largest eigenvalue of M_2 in modulus with, at a length scale L_n ,

$$\Delta_2(L_n) = \sum_{k=1}^{L_n} (\lambda_k - \bar{\lambda}) \sim \delta_2 \Omega_2^n \sim \delta_2 L_n^{\omega_2}. \tag{4.8}$$

Here, the amplitude of the perturbation δ_2 is a linear combination of coupling differences, $\lambda_{AA} - \lambda_{AB}$, $\lambda_{AA} - \lambda_{BA}$, ..., and the wandering exponent for bonds can be written as

$$\omega_2 = \frac{\ln |\Omega_2|}{\ln \Lambda_1}. \tag{4.9}$$

As a consequence, the wandering exponent changes when $|\Omega_2| = 1 > |\Lambda_2|$. Some examples are listed in the next section.

5. Relevance-irrelevance criterion

In both problems the aperiodic modulation introduces a thermal perturbation above $\bar{\lambda}$ which, at a length scale L , has an averaged density

$$\overline{\delta \lambda_i(L)} = \frac{\Delta_i(L)}{L} \sim \delta_i L^{\omega_i - 1} \quad i = 1, 2 \tag{5.1}$$

where the ω_i 's are the wandering exponents defined in (3.9) for the bond problem and (4.9) for the site problem.

Changing the length scale by $b = L/L'$ leads to the renormalized density

$$\overline{\delta \lambda'_i(L')} \sim \delta'_i \left(\frac{L}{b}\right)^{\omega_i - 1} = b^{1/\nu} \delta_i L^{\omega_i - 1} \quad i = 1, 2 \tag{5.2}$$

where ν is the bulk correlation length exponent. As a consequence, the perturbation amplitude δ_i transforms like

$$\delta'_i = b^{\omega_i - 1 + 1/\nu} \delta_i \tag{5.3}$$

with a crossover exponent $\Phi_i = 1 + \nu(\omega_i - 1)$ (Luck 1993a, Igló 1993).

When Φ_i is positive, the perturbation grows under rescaling, leading to a new fixed point with a different critical behaviour. When Φ_i is negative, the perturbation decays

under rescaling and the critical behaviour is the same as for the homogeneous system. The crossover exponent vanishes in the marginal case and then the critical exponents may vary continuously with the perturbation amplitude, i.e. the system may display a non-universal critical behaviour.

For the site problem, as mentioned at the end of section 2, the aperiodic modulation does not generally combine into a single effective parameter and one has to consider its effect on the transverse field and the two-spin interaction separately. The transverse field may take the values h_A or h_B like λ_k in the bond problem. Thus, the behaviour of the corresponding perturbation under rescaling is controlled by Φ_1 , whereas the perturbation of the two-spin interaction J_k is governed by Φ_2 . Since, according to the discussion of section 4, $\omega_2 \geq \omega_1$, for any singular quantity the critical behaviour will depend on the sign of Φ_2 in the site problem, as for the surface magnetization.

Table 2 gives the two largest eigenvalues of the substitution matrices and the wandering exponents for typical aperiodic sequences. For the two-dimensional Ising model with $\nu = 1$, the borderline between relevant and irrelevant behaviour corresponds to $\omega_i = 0$ according to (5.3). The bond and site aperiodic perturbations are irrelevant for the Fibonacci sequence, whereas the site perturbation becomes marginal for the Thue-Morse sequence. The following sequences all have divergent fluctuations so that the perturbation behaves in the same way for both problems. The period-doubling and three-folding sequences lead to marginal perturbations but the non-universal exponents should differ for the bond and site problems. The last sequence is relevant in both cases.

Table 2. Comparison between the bond and site problems for some typical sequences. The last two lines refer to the 2D Ising model.

Sequence	Fibonacci ^a	Thue-Morse ^b	Period-doubling ^c	Three-folding ^d	Fivefold ^e
$S\{A\}$	B	AB	BB	ABA	AAAB
$S\{B\}$	BA	BA	BA	ABB	BBA
Λ_1	τ^f	2	2	3	$2 + \tau$
$ \Lambda_2 $	$\tau - 1$	0	1	1	$3 - \tau$
$ \Omega_2 $	$\tau - 1$	1	1	1	$3 - \tau$
ω_1	-1	$-\infty$	0	0	0.25157
ω_2	-1	0	0	0	0.25157
Bond problem	Irrelevant	Irrelevant	Marginal	Marginal	Relevant
Site problem	Irrelevant	Marginal	Marginal	Marginal	Relevant

^a See e.g. Tracy (1988).

^b See e.g. Dekking *et al* (1983a).

^c This sequence appears in connection with the period-doubling cascade (Collet and Eckmann 1980).

^d This is the folding sequence of a dragon curve (Dekking *et al* 1983b).

^e This sequence is connected with tilings of the plane with fivefold symmetry (Godrèche and Luck 1992, Godrèche and Lançon 1992).

^f $\tau = (1 + \sqrt{5})/2$ is the golden mean.

6. General results: critical coupling and surface magnetization

The critical coupling of the inhomogeneous QIM is such that (Pfeuty 1979)

$$\lim_{L \rightarrow \infty} \prod_{k=1}^L \left(\frac{J_k}{h_k} \right)_c^{1/L} = \lim_{L \rightarrow \infty} \prod_{k=1}^L (\lambda_k)_c^{1/L} = 1. \quad (6.1)$$

For the bond problem, we take $\lambda_A = \lambda$ as a reference coupling and $\lambda_B = \lambda r$. We associate a digit f_k with the k th letter in the sequence. With $f_k = 0$ for A and $f_k = 1$ for B, the k th coupling can be written as $\lambda_k = \lambda r^{f_k}$. The critical coupling λ_c is such that $\lim_{L \rightarrow \infty} \lambda_c r^{n_L/L} = 1$ with

$$n_j = \sum_{k=1}^j f_k. \tag{6.2}$$

Finally, one obtains

$$\lambda_c = r^{-\rho_\infty} \tag{6.3}$$

where $\rho_\infty = \rho_\infty^B$ as defined in (3.6).

For the site problem, we take the following parametrization:

$$\lambda_{AA} = \lambda \quad \lambda_{AB} = \lambda u \quad \lambda_{BA} = \lambda v \quad \lambda_{BB} = \lambda r. \tag{6.4}$$

Due to the transverse field contribution, λ_{AB} is generally different from λ_{BA} . The effective coupling can be written as

$$\lambda_k = \lambda r^{f_k f_{k+1}} u^{f_{k+1} - f_k f_{k+1}} v^{f_k - f_k f_{k-1}} \tag{6.5}$$

and using (6.1), the critical coupling is such that

$$\lim_{L \rightarrow \infty} u^{(j_{L+1} - f_1)/L} \lambda_c s^{n_L/L} \left(\frac{r}{s}\right)^{m_L/L} = 1 \tag{6.6}$$

where $s = uv$ and

$$m_j = \sum_{k=1}^j f_k f_{k+1}. \tag{6.7}$$

The critical coupling is then given by

$$\lambda_c = s^{-\rho_\infty} \left(\frac{s}{r}\right)^{\kappa_\infty} \quad \kappa_\infty = \lim_{L \rightarrow \infty} \frac{m_L}{L}. \tag{6.8}$$

Alternatively, using the asymptotic densities defined in (4.4), the critical coupling can be expressed as

$$\lambda_c = u^{-\rho_\infty^{AB}} v^{-\rho_\infty^{BA}} r^{-\rho_\infty^{BB}}. \tag{6.9}$$

According to (2.5) and making use of (6.2) with $n_0 = 0$, the surface magnetization for the bond problem is given by

$$m_s = [S(\lambda, r)]^{-1/2} \quad S(\lambda, r) = \sum_{j=0}^{\infty} \lambda^{-2j} r^{-2n_j}. \tag{6.10}$$

For the site problem, using (2.5), (6.2), (6.5), and (6.7) with $m_0 = 0$, we have

$$m_s = [\Sigma(\lambda, r, s, u)]^{-1/2} \quad \Sigma(\lambda, r, s, u) = u^{2f_1} \sum_{j=0}^{\infty} \lambda^{-2j} \left(\frac{r}{s}\right)^{-2m_j} s^{-2n_j} u^{-2f_{j+1}}. \tag{6.11}$$

Since $f_k = 0, 1$, one may use the identity

$$a^{f_k} = 1 + (a - 1)f_k \tag{6.12}$$

to rewrite the sum as

$$\Sigma(\lambda, r, s, u) = u^{2f_1} \left[\Sigma_1 \left(\lambda, \frac{r}{s}, s \right) + (u^{-2} - 1)\Sigma_2 \left(\lambda, \frac{r}{s}, s \right) \right] \tag{6.13}$$

where

$$\Sigma_1(\lambda, x, y) = \sum_{j=0}^{\infty} \lambda^{-2j} x^{-2m_j} y^{-2n_j} \quad \Sigma_2(\lambda, x, y) = \sum_{j=0}^{\infty} \lambda^{-2j} x^{-2m_j} y^{-2n_j} f_{j+1}. \tag{6.14}$$

Let us consider the case $s=r$, i.e. $\lambda_{AB}\lambda_{BA} = \lambda_{AA}\lambda_{BB}$, a common approximation in the case of symmetric couplings ($\lambda_{AB} = \lambda_{BA}$). Then $\Sigma_1(\lambda, 1, r) = S(\lambda, r)$ and, using the identity $f_{j+1} = (r^{-2f_{j+1}} - 1)/(r^{-2} - 1)$, one obtains

$$\Sigma(\lambda, r, r, u) = u^{2(f_1-1)} \frac{1-u^2}{1-r^2} \left[\left(\lambda^2 r^2 + \frac{u^2-r^2}{1-u^2} \right) S(\lambda, r) - \lambda^2 r^2 \right]. \tag{6.15}$$

It follows that, for this particular combination of couplings, the critical behaviour is governed by $S(\lambda, r)$ and is the same as in the bond problem.

7. Period-doubling sequence

The results of the preceding sections will now be illustrated on the examples of two sequences with different surface magnetization exponents for the bond and site problems. We begin with the period-doubling sequence (Luck 1993a, Collet and Eckmann 1980) which is marginal for both problems, according to table 2.

Since the solution of the bond problem can be found elsewhere (Turban *et al* 1994), we only give a summary of the results. Starting the iteration on B and using the substitutions given in table 2, one obtains

$$\begin{aligned} & B \\ & B A \\ & B A B B \\ & B A B B B A B A \\ & B \underline{A} B \underline{B} B \underline{A} B \underline{A} B \underline{A} B \underline{B} B \underline{A} B \underline{B} \\ & \vdots \end{aligned} \tag{7.1}$$

The asymptotic density $\rho_{\infty} = \frac{2}{3}$ leads to the critical coupling

$$\lambda_c = r^{-2/3} \quad (\text{bond problem}). \tag{7.2}$$

The form of the substitution is such that

$$f_{2k} = 1 - f_k \quad f_{2k+1} = 1 \tag{7.3}$$

from which one deduces

$$n_{2j} = 2j - n_j \quad n_{2j+1} = 2j + 1 - n_j. \tag{7.4}$$

Splitting the sum $S(\lambda, r)$ in (6.10) into even and odd parts and using (7.4), one obtains the recursion relation

$$S(\lambda, r) = \left(1 + \frac{1}{\lambda^2 r^2}\right) S(\lambda^2 r^2, r^{-1}) \tag{7.5}$$

and the series can be written as an infinite product (Turban *et al* 1994)

$$S(\lambda, r) = \prod_{k=1}^{\infty} \left[1 + \lambda_c \left(\frac{\lambda_c}{\lambda}\right)^{2^{2k-1}}\right] \left[1 + \lambda_c^{-1} \left(\frac{\lambda_c}{\lambda}\right)^{2^{2k}}\right]. \tag{7.6}$$

Let $S(z)$ be the series expansion of $S(\lambda, r)$ in powers of $z = (\lambda_c/\lambda)^2$. According to (6.10), near the critical point $S(z)$ should display a power-law singularity with $S(z) \sim (1 - z)^{-2\beta_s}$, where β_s is the surface magnetization exponent. It may be shown that, at the critical point $z = 1$, the truncated series $S_L(z)$ containing the first L terms in $S(z)$ behaves as $L^{2\beta_s}$ (Iglói 1986). Since the first l terms in (7.6) just contain the truncated series with $L = 2^{2l}$, the surface magnetization exponent is given by (Turban *et al* 1994)

$$\beta_s = \frac{\ln[(1 + \lambda_c)(1 + \lambda_c^{-1})]}{4 \ln 2} = \frac{1}{2} \frac{\ln(\lambda_c^{1/2} + \lambda_c^{-1/2})}{\ln 2}. \tag{7.7}$$

Let us now consider the site problem. The critical coupling,

$$\lambda_c = (rs)^{-1/3} \quad (\text{site problem}) \tag{7.8}$$

follows from (4.4) and (6.9) with $\rho_{AB} = \rho_{BA} = \rho_{BB} = \frac{1}{3}$. Putting (7.3) into (6.7), one obtains the recursion relations

$$m_{2j} = 2j - 2n_j \quad m_{2j+1} = 2j + 1 - 2n_j - f_{j+1} \tag{7.9}$$

which can be used, together with those given in (7.4), to relate Σ_1 , Σ_2 and S . Splitting, as above, the sums in (6.14) into odd and even values of j , and using the identity

$$a^{f_k} = \frac{b - a}{b - 1} + \frac{a - 1}{b - 1} f_k \tag{7.10}$$

leads to

$$\begin{aligned} \Sigma_i(\lambda, x, y) &= a_i + b_i S[(\lambda xy)^2, (x^2 y)^{-1}] \quad i = 1, 2 \\ a_1 &= -(\lambda xy)^2 \frac{x^2 - 1}{x^4 y^2 - 1} \quad b_1 = 1 + (\lambda y)^{-2} \frac{x^2 y^2 - 1}{x^4 y^2 - 1} + (\lambda xy)^2 \frac{x^2 - 1}{x^4 y^2 - 1} \\ a_2 &= \frac{(\lambda xy)^2}{x^4 y^2 - 1} \quad b_2 = 1 + \frac{\lambda^{-2} x^2 - (\lambda xy)^2}{x^4 y^2 - 1}. \end{aligned} \tag{7.11}$$

These relations, with $x = r/s$, $y = s$, and (6.13), with $f_1 = 1$, finally give

$$\begin{aligned} \Sigma(\lambda, r, s, u) &= a + bS \left[\lambda^2 r^2, \frac{s}{r^2} \right] \\ a &= \lambda^2 r^2 \frac{s^2 - r^2 u^2}{r^4 - s^2} \\ b &= 1 + \frac{\lambda^{-2}(r^2 - u^2) + \lambda^2 r^2 (r^2 u^2 - s^2)}{r^4 - s^2} \end{aligned} \quad (7.12)$$

which, together with (7.6), solves the site problem. Some examples of the temperature variation of the surface magnetization are shown in figures 1 and 2. Similar curves, for the bond problem, can be found in Turban *et al* (1994).

The critical behaviour of the surface magnetization for the site problem is governed by the singularity of $S(\lambda', r')$ in (7.12), at λ'_c given by (7.2), with $\lambda' = \lambda^2 r^2$, $r' = sr^{-2}$. It follows that the critical coupling satisfies $\lambda_c^2 r^2 = (sr^{-2})^{-2/3}$, in agreement with (7.8). Changing λ_c into $\lambda'_c = (sr^{-2})^{-2/3}$ in (7.7), one obtains the surface magnetization exponent for the site problem

$$\beta_s = \frac{1}{2} \frac{\ln \left[(r^2 s^{-1})^{1/3} + (r^2 s^{-1})^{-1/3} \right]}{\ln 2}. \quad (7.13)$$

When $r = s$, the critical exponent is the same as for the bond problem in (7.7), as shown in section 6. The variation with r^2/s is shown in figure 3. One may notice that the value $\beta_s = \frac{1}{2}$, corresponding to the surface exponent of the homogeneous two-dimensional Ising model at the ordinary surface transition, is recovered when $s = uv = r^2$ and $\lambda_c = r^{-1}$. This result is linked to the absence of AA pairs in the sequence. This value is also the minimum value of the exponent β_s , i.e. the aperiodicity generally weakens the singularity.

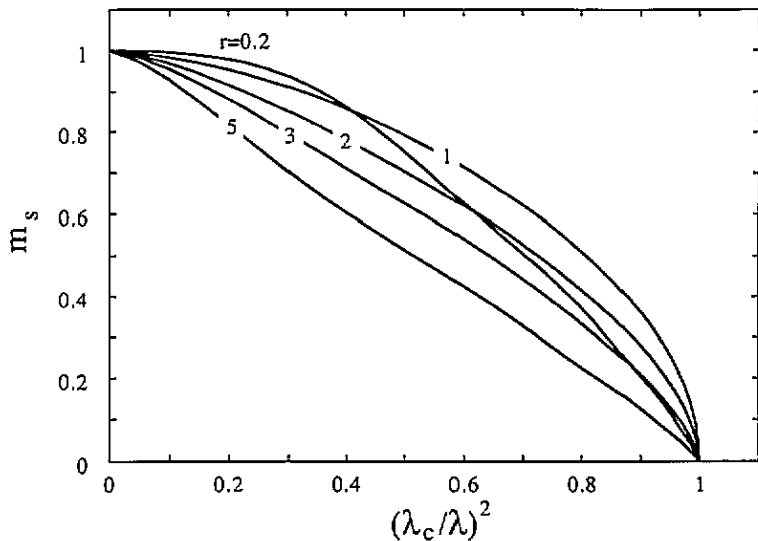


Figure 1. Temperature dependence of the surface magnetization (period-doubling, site problem) for different values of r , $u = 0.5$ and $v = 2$.

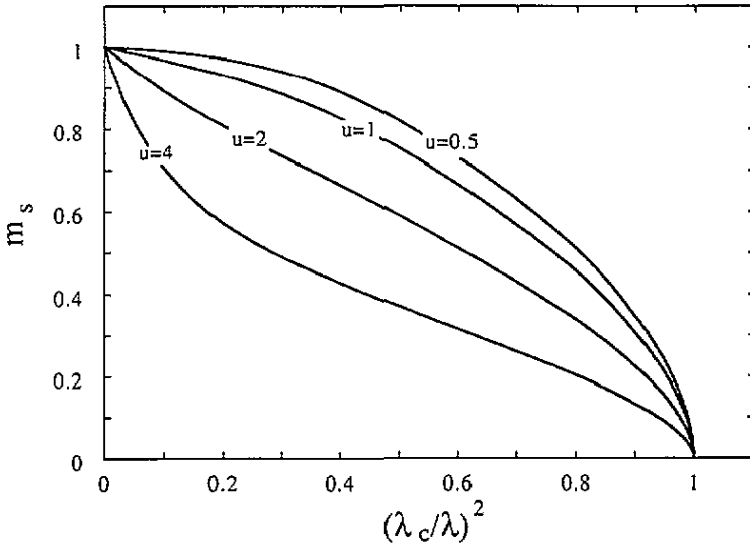


Figure 2. Temperature dependence of the surface magnetization (period-doubling, site problem) for different values of u , $r=0.5$ and $s=1$.

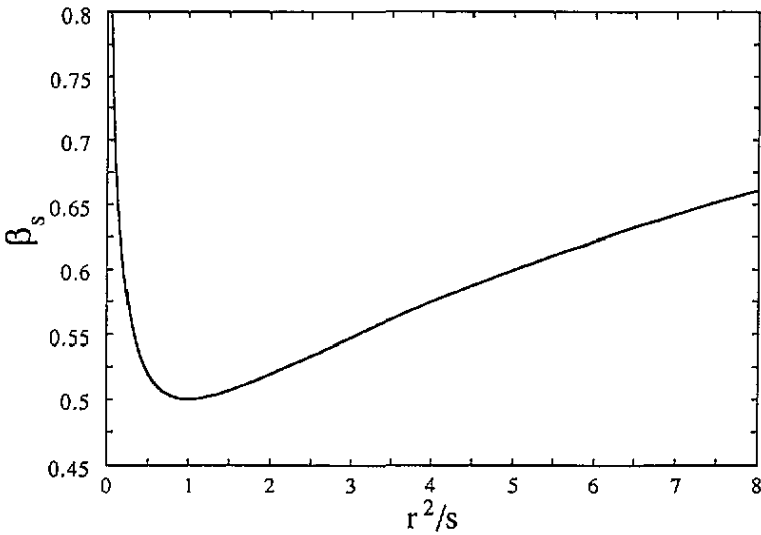


Figure 3. Variation of the surface magnetization exponent with r^2/s in the site problem for the period-doubling sequence.

8. Thue–Morse sequence

As a second example, we consider the binary Thue–Morse sequence (Dekking *et al* 1983a), which, as mentioned in table 2, leads to an irrelevant perturbation for the bond problem, treated in Turban *et al* (1994), and to a marginal one for the site problem. Starting with the letter A, the Thue–Morse substitution in table 2 gives, successively,

$$\begin{aligned}
 &A \\
 &A B \\
 &A B B A \\
 &A B B A B A A B \\
 &\underline{A} B \underline{B} A \underline{B} A \underline{A} B \underline{B} A \underline{A} B \underline{A} B \underline{A} B \underline{B} A \\
 &\vdots
 \end{aligned} \tag{8.1}$$

In the bond problem, the critical coupling

$$\lambda_c = r^{-1/2} \quad (\text{bond problem}) \tag{8.2}$$

follows from the asymptotic density $\rho_\infty = \frac{1}{2}$ given by (3.6). The form of the substitutions immediately leads to the recursion relations

$$f_{2k} = 1 - f_k \quad f_{2k+1} = f_{k+1} \tag{8.3}$$

which can be used in (6.2) to give

$$n_{2j} = j \quad n_{2j+1} = j + f_{j+1}. \tag{8.4}$$

A chain with length $L = 2j$ has a density equal to the asymptotic one, which explains the vanishing second eigenvalue Λ_2 in table 2.

Since the calculation of m_s has already been described elsewhere (Turban *et al* 1994), we just mention the results. The surface magnetization follows from

$$\begin{aligned}
 S(\lambda, r) &= \frac{1+r(\lambda_c/\lambda)^2}{1-(\lambda_c/\lambda)^4} + (r^{-1}-r)\left(\frac{\lambda}{\lambda_c}\right)^2 S_{\text{TM}}\left[\left(\frac{\lambda_c}{\lambda}\right)^4\right] \\
 S_{\text{TM}}(x) &= x \sum_{k=0}^{\infty} \frac{x^{2^k} \prod_{p=0}^k (1-x^{2^p})}{(1-x^{2^k})(1-x^{2^{k+1}})}
 \end{aligned} \tag{8.5}$$

where $S_{\text{TM}}(x) = \sum_{k=1}^{\infty} f_k x^k$ is the Thue–Morse series (Dekking *et al* 1983a). Near the critical point, one obtains

$$m_s = \frac{2t^{1/2}}{\lambda_c + \lambda_c^{-1}} \left[1 + \frac{1}{4} \left(\frac{1 - \lambda_c^2}{1 + \lambda_c^2} \right)^2 t + O(t^2) \right] \tag{8.6}$$

where $t = 1 - (\lambda_c/\lambda)^2$ is the deviation from the critical point. The surface magnetization exponent takes its unperturbed value, $\beta_s = \frac{1}{2}$, as expected for an irrelevant perturbation.

In the site problem, with $\rho_\infty^{\text{AA}} = \rho_\infty^{\text{BB}} = \frac{1}{6}$ and $\rho_\infty^{\text{AB}} = \rho_\infty^{\text{BA}} = \frac{1}{3}$, the critical coupling takes the form

$$\lambda_c = r^{-1/6} s^{-1/3} \quad (\text{site problem}). \tag{8.7}$$

Making use of (8.3), equation (6.7) leads to

$$m_{2j} = m_{2j+1} = n_{j+1} - m_j. \tag{8.8}$$

The same result is obtained for even and odd terms because the two letters occur within successive pairs along the sequence, so that $f_{2k+1}f_{2k+2}=0$.

With a sequence starting on A, the front factor disappears in the sum $\Sigma(\lambda, r, s, u)$ of (6.13). The Σ_i 's, defined in (6.14), satisfy the functional equations

$$\begin{aligned}\Sigma_i(\lambda, x, y) &= \sum_{j=1,2} a_{ij} \Sigma_j(\lambda^2 y, x^{-1}, x) \quad i = 1, 2 \\ a_{11} &= 1 + \lambda^{-2} \quad a_{12} = x^{-2} - \lambda^{-2} + (\lambda x y)^{-2} - 1 \\ a_{21} &= \lambda^{-2} \quad a_{22} = x^{-2} - \lambda^{-2}\end{aligned}\tag{8.9}$$

which, as usual, are obtained by splitting the sums into even and odd parts and using (8.4), (8.8), as well as the identity (6.12).

Through iteration, at step $k \geq 1$, the arguments of the Σ_i s become

$$\lambda_k = \lambda^{2^k} x^{[2^{k-1} + (-1)^k]/3} y^{2^{k-1}} \quad x_k = y_k^{-1} = x^{(-1)^k}\tag{8.10}$$

and the functional equations (8.9) can be rewritten in matrix form as

$$\begin{pmatrix} \Sigma_1(\lambda_k, x_k, y_k) \\ \Sigma_2(\lambda_k, x_k, y_k) \end{pmatrix} = \mathbf{T}_k \begin{pmatrix} \Sigma_1(\lambda_{k+1}, x_{k+1}, y_{k+1}) \\ \Sigma_2(\lambda_{k+1}, x_{k+1}, y_{k+1}) \end{pmatrix}\tag{8.11}$$

with

$$\mathbf{T}_k = \begin{pmatrix} 1 + \lambda_k^{-2} & x_k^{-2} - 1 \\ \lambda_k^{-2} & x_k^{-2} - \lambda_k^{-2} \end{pmatrix} \quad k \geq 1.\tag{8.12}$$

Then,

$$\begin{pmatrix} \Sigma_1(\lambda_1, x_1, y_1) \\ \Sigma_2(\lambda_1, x_1, y_1) \end{pmatrix} = \prod_{k=1}^{\infty} \mathbf{T}_k \begin{pmatrix} 1 \\ 0 \end{pmatrix}\tag{8.13}$$

where the components of the vector on the right follows from the form of the Σ_i 's when $k \rightarrow \infty$.

Equations (6.11), (6.13), and (8.11)–(8.13), formally solve the problem. The temperature variation of the surface magnetization is shown in figures 4 and 5.

It seems difficult to obtain an explicit expression for the surface magnetization since the form of the matrix \mathbf{T}_k depends on the index k . But some progress can be made concerning the critical behaviour, using the same scaling method as for the period-doubling sequence, i.e. looking at the L dependence of the truncated series $\Sigma_L(z)$ at the critical point $z = (\lambda_c/\lambda)^2 = 1$.

With the actual values of the arguments in (6.13), $x = r/s$ and $y = s$, equation (8.10) gives

$$\lambda_k = \left(\frac{r}{s}\right)^{(-1)^k/3} \left(\frac{\lambda}{\lambda_c}\right)^{2^k} \quad x_k = y_k^{-1} = \left(\frac{r}{s}\right)^{(-1)^k}\tag{8.14}$$

so that, at the critical point, the matrix elements in \mathbf{T}_k depend on k only through $(-1)^k$. Let us introduce the product $\mathbf{U} = \mathbf{T}_{2p-1} \mathbf{T}_{2p}$ with

$$\mathbf{U} = \begin{pmatrix} 2 + w + w^2 & (w^{-1} - w)(1 + w + w^{-1}) \\ w + w^2 & (1 - w)(2 + w) \end{pmatrix} \quad w = \left(\frac{r}{s}\right)^{2/3}.\tag{8.15}$$

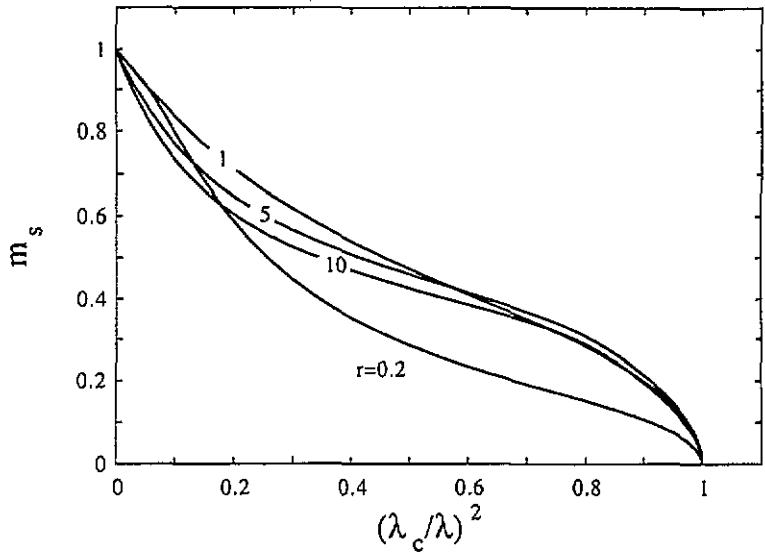


Figure 4. Temperature dependence of the surface magnetization (Thue-Morse, site problem) for different values of r , $\mu=0.5$ and $s=1$.

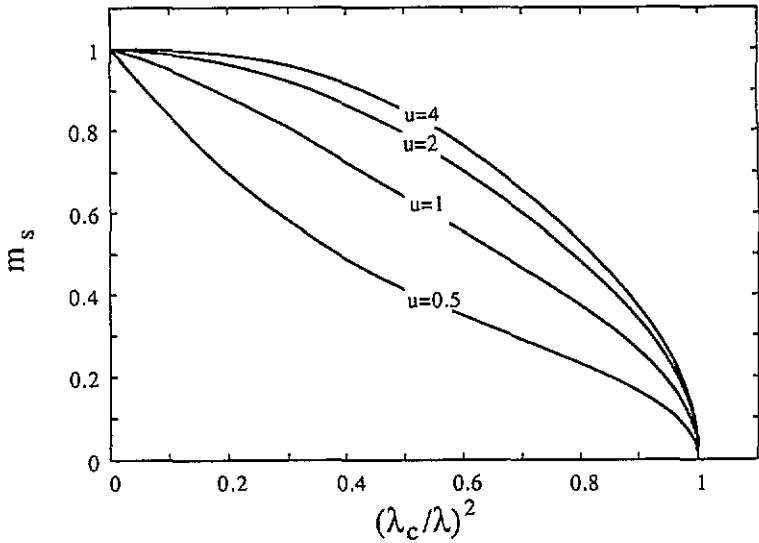


Figure 5. Temperature dependence of the surface magnetization (Thue-Morse, site problem) for different values of u , $r=0.5$ and $s=1$.

Taking $L=2^{2l}$, the first L terms in $\Sigma_L(z)$ are obtained, up to L -independent factors, keeping the first $2l$ terms in the infinite product of (8.13). Due to the form of the matrix elements in (8.12), they belong to the first column of the matrix resulting from the finite product. Thus, using (8.15), they are also given by $\mathbf{U}^l \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ at the critical point. After diagonalization, one obtains

$$\Sigma_L(1) \sim (2^{2l})^{2\beta_s} \sim (w^{1/4} + w^{-1/4})^{2l} \tag{8.16}$$

where the last term is the l th power of the largest eigenvalue of \mathbf{U} . Finally, the surface magnetization exponent reads

$$\beta_s = \frac{1}{2} \frac{\ln [(rs^{-1})^{1/6} + (rs^{-1})^{-1/6}]}{\ln 2}. \quad (8.17)$$

The surface magnetization exponent is shown as a function of r/s in figure 6. The minimum value $\beta_s = \frac{1}{2}$, corresponding to the homogeneous system and to the bond problem behaviour as well, is reached when $r = s$.

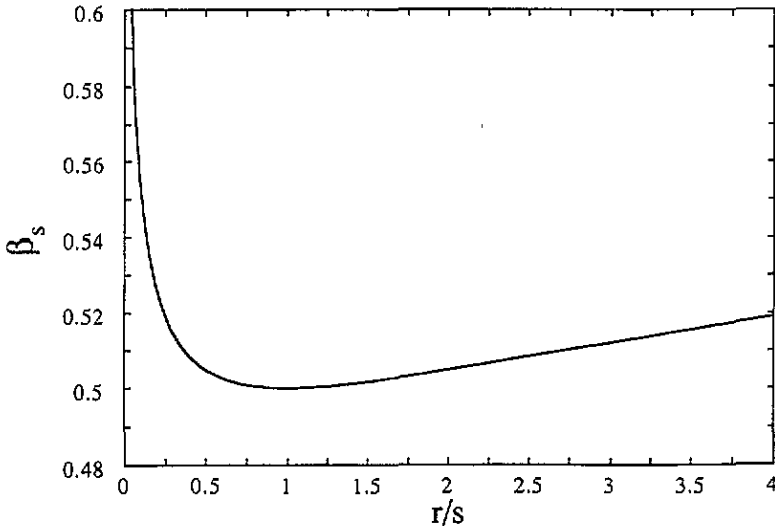


Figure 6. Variation of the surface magnetization exponent with r/s in the site problem for the Thue–Morse sequence.

9. Conclusion

We have presented a comparative study of the influence of bond and site aperiodicities on the critical behaviour at a second-order phase transition. One-dimensional sequences generated through substitution, corresponding to an uniaxial aperiodic modulation, have been discussed. The extension of the Harris criterion to the site problem requires the knowledge of the eigenvalues of a substitution matrix which is linked to the distribution of pairs of successive letters along the sequence. For sequences with $|\Lambda_2| \geq 1$, the relevance–irrelevance criterion is the same in the bond and site problems. When $|\Lambda_2| < 1$, the aperiodic perturbation may become more dangerous in the site problem, depending on the form of the substitution.

Exact results have been obtained for the surface magnetization of layered Ising aperiodic systems. The period-doubling sequence leads to a marginal perturbation for both problems, but with different non-universal exponents. The Thue–Morse aperiodic modulation, which is irrelevant for the bond problem, becomes marginal for the site problem, where the surface magnetic exponent is non-universal.

Among the possible extensions of this work, one may mention the treatment of substitutions with more than two letters and, more interesting, the study of higher-dimensional aperiodic perturbations in isotropic or anisotropic critical systems.

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