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Aperiodic spin chain in the mean field approximation

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Received 15 July 1996

Abstract. Surface and bulk critical properties of an aperiodic spin chain are investigated in the framework of the ϕ^4 phenomenological Ginzburg–Landau theory. According to Luck’s criterion, the mean field correlation length exponent $\nu = \frac{1}{2}$ leads to a marginal behaviour when the wandering exponent of the sequence is $\omega = -1$. This is the case of the Fibonacci sequence that we consider here. We calculate the bulk and surface critical exponents for the magnetizations, critical isotherms, susceptibilities and specific heats. These exponents continuously vary with the amplitude of the perturbation. Hyperscaling relations are used in order to obtain an estimate of the upper critical dimension for this system.

1. Introduction

The discovery of quasicrystals [1] has focused considerable interest on quasiperiodic or, more generally, aperiodic systems [2]. In the field of critical phenomena, due to their intermediate situation between periodic and random systems, aperiodic models have been intensively studied (for a review, see [3]). Furthermore, aperiodic multilayers are experimentally feasible and should build a new class of artificial structures exhibiting interesting bulk and surface properties. Although aperiodic superlattices have already been worked out by molecular beam epitaxy [4], nothing experimental has been done up to now from the point of view of critical phenomena. In the perspective of possible future experimental studies in this context, it seems an interesting and challenging problem to complete our understanding through a mean field theory approach. Surface critical behaviour has indeed been intensively investigated on the basis of the Ginzburg–Landau theory [5] in the 1970s [6]. This led to a classification of the transitions which may occur at the surface and to the derivation of scaling laws between surface and bulk critical exponents [7] (for a review, see [8]). These early papers are known as an important stage in the further developments of surface critical phenomena.

From the point of view of critical phenomena, the universal behaviour of aperiodically perturbed systems is now well understood since Luck proposed a relevance–irrelevance criterion [9, 10]. The characteristic length scale in a critical system is given by the correlation length and, as in the Harris criterion for random systems [11], the strength of the fluctuations of the couplings on this scale determines the critical behaviour. An aperiodic perturbation can thus be relevant, marginal or irrelevant, depending on the sign of a crossover exponent involving the correlation length exponent ν of the unperturbed system and the wandering

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exponent ω which governs the size-dependence of the fluctuations of the aperiodic couplings [12]. In the light of this criterion, the results obtained in early papers, mainly concentrated on the Fibonacci [13] and the Thue–Morse [14] sequences, found a consistent explanation, since, resulting from the bounded fluctuations, a critical behaviour which resembles the periodic case was found for the Ising model in two dimensions.

In recent years, much progress has been made in the understanding of the properties of marginal and relevant aperiodically perturbed systems. Exact results for the $2d$ layered Ising model and the quantum Ising chain have been obtained with irrelevant, marginal and relevant aperiodic perturbations [15, 16]. The critical behaviour is in agreement with Luck's criterion leading to essential singularities or first-order surface transition when the perturbation is relevant and power laws with continuously varying exponents in the marginal situation with logarithmically diverging fluctuations. A strongly anisotropic behaviour has been recognized in this latter situation [17, 18]. Marginal surface perturbations have also been studied with the Fredholm sequence [19] and conformal aspects have been discussed [20].

In the present paper, we continue our study of marginal sequences. The case of the Fibonacci sequence, which leads to irrelevant behaviour in the Ising model, should exhibit non-universal properties within the mean field approach according to the Luck criterion and it has not yet been studied in this context. The article is organized as follows. In section 2, we present the phenomenological Ginzburg–Landau theory on a discrete lattice with a perturbation following a Fibonacci sequence and we summarize the scaling arguments leading to Luck's criterion, then we discuss the definitions of both bulk and surface thermodynamic quantities. In section 3 we consider magnetic properties; both bulk and surface quantities are computed numerically, leading to the values of the corresponding critical exponents. In section 4, we discuss the thermal properties and eventually in section 5, we discuss the upper critical dimension of the model.

2. Discrete Ginzburg–Landau equations for a Fibonacci aperiodic perturbation

2.1. Landau expansion and equation of state on a one-dimensional lattice

Let us first briefly review the essentials of the Ginzburg–Landau theory formulated on a discrete lattice. We consider a one-dimensional lattice of L sites with a lattice spacing ℓ and free boundary conditions. The critical behaviour would be the same as in a d -dimensional plate of thickness $L\ell$ with translational invariance along the $d - 1$ directions perpendicular to the chain and extreme axial anisotropy which forces the magnetic moments to keep a constant direction in the plane of the plate. We investigate the critical properties of an aperiodically distributed perturbation within the framework of a ϕ^4 phenomenological Landau theory [21]. The underlying assumption in this approach is based on the following expansion of the bulk free energy density

$$f_b\{\phi_j\} = \frac{1}{2}\mu_j\phi_j^2 + \frac{1}{4}g\phi_j^4 - H\phi_j + \frac{1}{2}c\left(\frac{\phi_{j+1} - \phi_j}{\ell}\right)^2 \quad (1)$$

where the aperiodic perturbation of the coupling constants is determined by a two-digits substitution rule and enters the ϕ^2 term only. A dimensional analysis indeed shows that the deviation from the critical temperature, μ , is the relevant scaling field which has to be modified by the perturbation. The free energy of the whole chain is thus given by

$$F[\phi_j] = \sum_j f_b\{\phi_j\} \quad (2)$$

and the spatial distribution of order parameter satisfies the usual functional minimization

$$\delta F[\phi_j] = F[\phi_j + \delta\phi_j] - F[\phi_j] = 0. \tag{3}$$

One then obtains the coupled discrete Ginzburg–Landau equations

$$\mu_j\phi_j + g\phi_j^3 - H - \frac{c}{\ell^2}(\phi_{j+1} - 2\phi_j + \phi_{j-1}) = 0. \tag{4}$$

The coefficients μ_j depend on the site location and are written as

$$\mu_j = k_B T - (zJ - Rf_j) = a_0 \left(1 - \frac{1}{\theta} + rf_j \right) \tag{5}$$

where J is the exchange coupling between neighbour sites in the homogeneous system, z is the lattice coordination and f_j is the aperiodically distributed sequence of 0 and 1. The prefactor $a_0 = k_B T$ is essentially constant in the vicinity of the critical point, and the temperature θ is normalized relatively to the unperturbed system critical temperature: $\theta = k_B T / zJ$. In the following, we will also use the notation $\mu = 1 - 1/\theta$. In order to obtain a dimensionless equation, let us define $\phi_j = m_j \sqrt{a_0/g}$ leading to the following nonlinear equations for the m_j 's

$$(\mu + rf_j)m_j + m_j^3 - h - (m_{j+1} - 2m_j + m_{j-1}) = 0 \tag{6}$$

with boundary conditions

$$(\mu + rf_1)m_1 + m_1^3 - h - (m_2 - 2m_1) = 0 \tag{7a}$$

$$(\mu + rf_L)m_L + m_L^3 - h - (-2m_L + m_{L-1}) = 0. \tag{7b}$$

Here, the lengths are measured in units of $\ell = \sqrt{c/a_0}$ and $h = H\sqrt{g/a_0^3}$ is a reduced magnetic field.

One can point out the absence of a specific surface term in the free energy density. The surface equations for the order parameter profile simply keep the bulk form with the boundary conditions $m_0 = m_{L+1} = 0$ and our study will only concern ordinary surface transitions [8].

2.2. *Fibonacci perturbation and Luck's criterion*

The Fibonacci perturbation considered below may be defined as a two-digits substitution sequence which follows from the inflation rule

$$0 \rightarrow S(0) = 01 \quad 1 \rightarrow S(1) = 0 \tag{8}$$

leading, by iterated application of the rule on the initial word 0, to successive words of increasing lengths

$$\begin{array}{cccccccc} 0 & & & & & & & & \\ 0 & 1 & & & & & & & \\ 0 & 1 & 0 & & & & & & \\ 0 & 1 & 0 & 0 & 1 & & & & \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & \\ \dots & & & & & & & & \end{array} \tag{9}$$

It is now well known that most of the properties of such a sequence can be characterized by a substitution matrix whose elements, M_{ij} , are given by the number, $n_i^{S(j)}$, of digits of type i in the substitution $S(j)$ [9, 12]. In the case of the Fibonacci sequence, this yields

$$\mathbf{M} = \begin{pmatrix} n_0^{S(0)} & n_0^{S(1)} \\ n_1^{S(0)} & n_1^{S(1)} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \quad (10)$$

The largest eigenvalue of the substitution matrix is given by the golden mean $\Lambda_1 = \frac{1+\sqrt{5}}{2}$ and is related to the length of the sequence after n iterations, $L_n \sim \Lambda_1^n$, while the second eigenvalue $\Lambda_2 = -1/\Lambda_1$ governs the behaviour of the cumulated deviation from the asymptotic density of modified couplings $\rho_\infty = 1 - \frac{2}{\sqrt{5}+1}$

$$\sum_{j=1}^L (f_j - \bar{f}) = n_L - \rho_\infty L \sim |\Lambda_2|^n \sim (\Lambda_1^\omega)^n \quad (11)$$

where we have introduced the sum $n_L = \sum_{j=1}^L f_j$ and the wandering exponent

$$\omega = \frac{\ln |\Lambda_2|}{\ln \Lambda_1} = -1. \quad (12)$$

When the scaling field μ is perturbed as considered in the previous section,

$$\mu_j = a_0(\mu + r f_j) \quad (13)$$

the cumulated deviation of the couplings from the average at a length scale L

$$\overline{\delta\mu}(L) = \frac{1}{L} \sum_{j=1}^L (\mu_j - \bar{\mu}) = \frac{1}{L} a_0 r (n_L - \rho_\infty L) \quad (14)$$

behaves with a size power law

$$\overline{\delta\mu}(L) \sim L^{\omega-1} \quad (15)$$

and induces a shift in the critical temperature $\overline{\delta t} \sim \xi^{\omega-1}$ to be compared with the deviation t from the critical temperature

$$\frac{\overline{\delta t}}{t} \sim t^{-(\nu(\omega-1)+1)}. \quad (16)$$

This defines the crossover exponent $\phi = \nu(\omega - 1) + 1$. When $\phi = 0$, the perturbation is marginal: it remains unchanged under a renormalization transformation, and the system is thus governed by a new perturbation-dependent fixed point.

A perturbation of the parameters g or c entering the Landau expansion (1) would be irrelevant.

2.3. Bulk and surface thermodynamic quantities

In the following, we discuss both bulk and surface critical exponents and scaling functions. We deal with the surface and boundary magnetizations m_s and m_1 , surface and boundary susceptibilities χ_s and χ_1 , and surface specific heat C_s . All these quantities can be expressed as derivatives of the surface free energy density f_s [8] (see table 1).

While there is no need to pay special attention to these definitions in a homogeneous system, they have to be carefully rewritten in the perturbed model that we consider here. First of all, we shall focus on local quantities such as the boundary magnetization m_1 or the local bulk magnetization $m_{(n-1)}$, defined, for a chain of size L_n obtained after n

Table 1. Bulk and surface thermodynamic quantities in terms of the bulk f_b and surface f_s free energy densities. h and h_1 are bulk and surface magnetic fields respectively and t is the reduced temperature.

| Magnetization | | Susceptibility | | Specific heat | |
|------------------------------------------|----------------------------------------------------------------------------------------|-------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|----------------------------------------------|
| Bulk | Surface | Bulk | Surface | Bulk | Surface |
| $m_b = -\frac{\partial f_b}{\partial h}$ | $m_s = -\frac{\partial f_s}{\partial h}$ $m_1 = -\frac{\partial f_s}{\partial h_1}$ | $\chi_b = -\frac{\partial^2 f_b}{\partial h^2}$ | $\chi_s = -\frac{\partial^2 f_s}{\partial h^2}$ $\chi_1 = -\frac{\partial^2 f_s}{\partial h \partial h_1}$ $\chi_{11} = -\frac{\partial^2 f_s}{\partial h_1^2}$ | $C_b = -\frac{\partial^2 f_b}{\partial t^2}$ | $C_s = -\frac{\partial^2 f_s}{\partial t^2}$ |

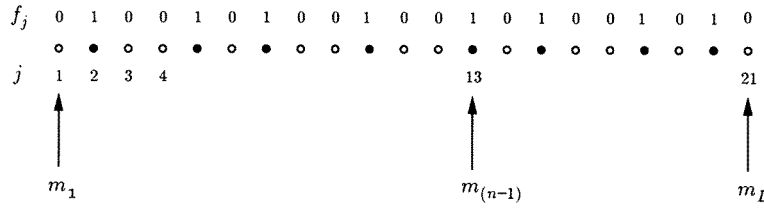


Figure 1. Fibonacci chain of 21 sites. The local bulk magnetization, for a chain of L_n sites obtained after n iterations of the substitution rule is computed on the site L_{n-1} , here site 13.

substitutions, by the order parameter at position L_{n-1} . This definition leads to equivalent sites for different chain sizes (see figure 1).

In addition to these local quantities, one may also calculate both surface and mean bulk magnetizations (m_s and m_b respectively), which should be interesting from an experimental point of view since any experimental device would average any measurement over a large region compared with a microscopic scale. In order to keep symmetric sites with respect to the middle of the chain, and to avoid surface effects, the mean bulk magnetization m_b is defined by averaging over L_{n-2} sites around the middle for a chain of size L_n

$$m_b = \frac{1}{L_{n-2}} \sum_{j \in L_{n-2}} m_j. \tag{17}$$

We numerically checked that one recovers the same average as for a chain of size L_{n-2} with periodic boundary conditions. Following Binder [8], for a film of size L_n with two free surfaces, the surface magnetization is then defined by the deviation of the average magnetization $\langle m_j \rangle$ over the whole chain from the bulk mean value

$$m_s = \frac{1}{2} \left(m_b - \frac{1}{L_n} \sum_{j=1}^{L_n} m_j \right). \tag{18}$$

A graphical description can be found in figure 2.

In the following, we shall use brackets for the averages over the finite system, taking thus surface effects into account. In the same way, the bulk free energy density in table 1 has to be understood as

$$f_b = \frac{1}{L_{n-2}} \sum_{j \in L_{n-2}} f_b \{m_j\} \tag{19}$$

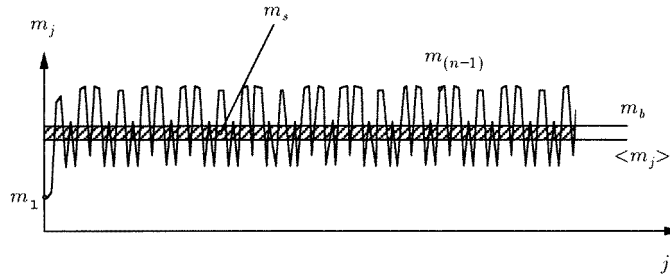


Figure 2. Typical shape of the order parameter profile for a perturbed system, showing the boundary and local bulk magnetizations m_1 and $m_{(n-1)}$, and the average values m_b and $\langle m_j \rangle$.

while the surface free energy density, f_s , is defined as the excess from the average bulk free energy

$$F = \sum_{j=1}^{L_n} f_b\{m_j\} = L_n \langle f_b \rangle = L_n f_b + 2f_s. \quad (20)$$

3. Magnetic properties

3.1. Order parameter profile and critical temperature

The order parameter profile is determined numerically by a Newton–Raphson method, starting with arbitrary values for the initial trial profile m_j . Equation (6) provides a system of L -coupled nonlinear equations

$$G_i(m_1, m_2, \dots, m_L) = 0 \quad i = 1, 2, \dots, L \quad (21)$$

for the components of the vector $\mathbf{m} = (m_1, m_2, \dots, m_L)$, which can be expanded in a first-order Taylor series

$$G_i(\mathbf{m} + \delta\mathbf{m}) = G_i(\mathbf{m}) + \sum_{j=1}^L \frac{\partial G_i}{\partial m_j} \delta m_j + O(\delta\mathbf{m}^2). \quad (22)$$

A set of linear equations follows for the corrections $\delta\mathbf{m}$

$$\sum_{j=1}^L \frac{\partial G_i}{\partial m_j} \delta m_j = -G_i(\mathbf{m}) \quad (23)$$

which moves each function G_i closer to zero simultaneously. This technique is known to provide a fast convergence towards the exact solution. Typical examples of the profile obtained for the Fibonacci perturbation are shown in figure 3.

The magnetization profile decreases as the temperature is increased and vanishes for some size-dependent effective value of the critical temperature $\mu_c(L) = 1 - (\theta_c(L))^{-1}$. This value may be obtained through a recursion relation deduced from the equation of state. In the high temperature phase, when $h = 0$, equation (6) can be rewritten as a homogeneous

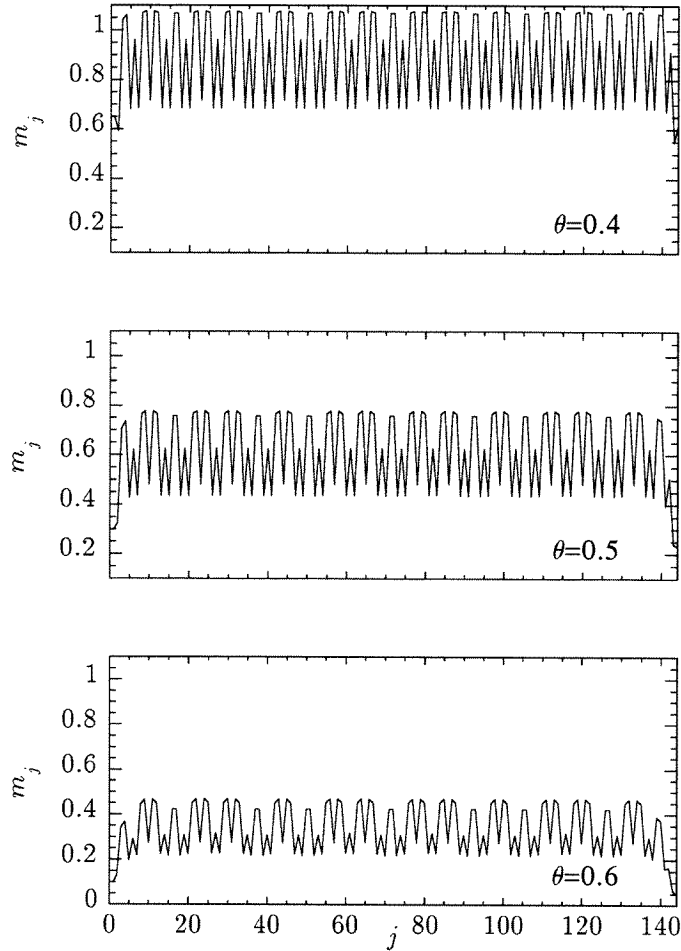


Figure 3. Order parameter profiles for a perturbation $r = 2$ and three values of the temperature below the critical point. The size of the chain is $L = 144$.

system of linear equations

$$\mathbf{G}\mathbf{m} = \begin{pmatrix} \alpha_1 & -1 & 0 & 0 & \dots & 0 \\ -1 & \alpha_2 & -1 & 0 & \dots & 0 \\ 0 & -1 & \alpha_3 & -1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \alpha_j & \ddots & \vdots \\ 0 & \dots & 0 & 0 & -1 & \alpha_L \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_L \end{pmatrix} = 0 \tag{24}$$

where $\alpha_j = 2 + \mu + rf_j$. If the determinant $D_L(\mu) = \text{Det } \mathbf{G}(\mu)$ is not vanishing, the null vector $\mathbf{m} = \mathbf{0}$ provides the satisfying unique solution for the high temperature phase. The critical temperature is then defined by the limiting value $\mu_c(L)$ which allows a non-vanishing solution for \mathbf{m} , i.e. $D_L(\mu_c) = 0$. Because of the tridiagonal structure of the

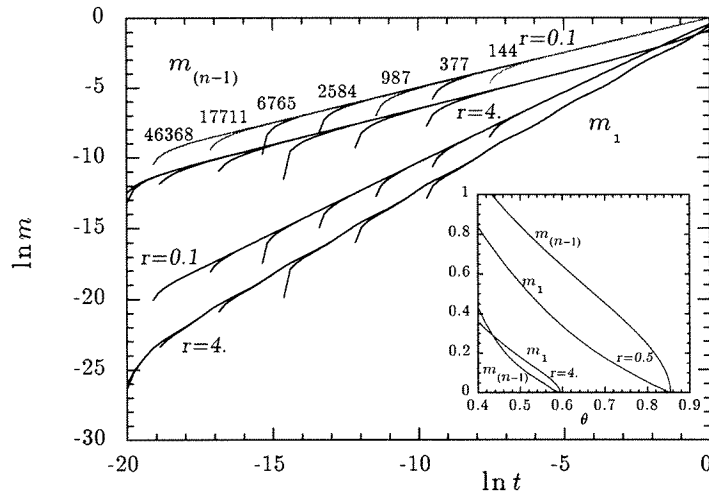


Figure 4. Log-log plot of the bulk and boundary magnetization versus the reduced temperature $t = \mu_c - \mu$ for two values of the aperiodic amplitude r and for different sizes of the chain from 144 to 46 368. Finite-size effects occur when the curves deviate from the asymptotic straight line. The insert shows the behaviour of the magnetization with the temperature.

determinant, the following recursion relation holds, for any value of μ

$$D_L(\mu) = \alpha_L D_{L-1}(\mu) - D_{L-2}(\mu) \quad (25a)$$

$$D_0(\mu) = 1 \quad (25b)$$

$$D_1(\mu) = \alpha_1. \quad (25c)$$

Thus, we can obtain $\mu_c(L)$ for different sizes of L , from 144 to 46 368 and estimate the asymptotic critical point by an extrapolation to infinite size. This technique allows a determination of the critical temperature with an absolute accuracy in the range 10^{-7} – 10^{-9} depending on the value of the amplitude r .

3.2. Surface and bulk spontaneous magnetization behaviours

The boundary magnetization m_1 vanishes at the same temperature as the profile itself. First of all, the influence of finite size effects [22] has to be studied. This is done by the determination of the profiles for different lengths of chains given by the successive sizes of the Fibonacci sequence $L = 1, 2, 3, 5, 8, 13, 21, 34, \dots$. The boundary and bulk magnetization in zero magnetic field are shown in figure 4 on a log-log scale.

The finite size effects appear in the deviation from the straight line asymptotic behaviour. These effects are not too sensitive, as it can be underscored by considering the deviation of the curve for a size $L = 17 711$, which occurs around $t = \mu_c - \mu \simeq 10^{-7}$, i.e. very close to the critical point.

The expected marginal behaviour is furthermore indicated by the variation of the slopes with the aperiodic modulation amplitude r and is more noticeable for the boundary magnetization than in the case of the bulk.

A more detailed inspection of these curves also shows oscillations resulting from the discrete scale invariance [23] of the system and the asymptotic magnetization can thus be written

$$m(t) = t^\beta \tilde{m}(t^{-\nu}) \quad (26)$$

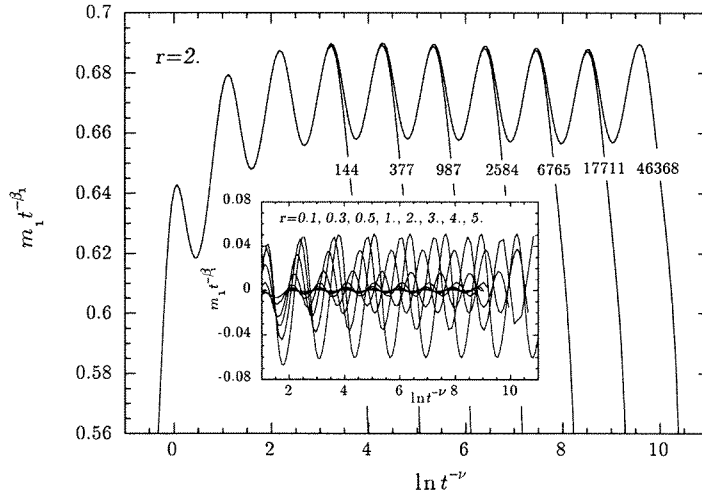


Figure 5. Periodic oscillations of the rescaled boundary magnetization $m_1 t^{-\beta_1}$ versus $\ln t^{-\nu}$. The deviation from the oscillating behaviour for large values of the correlation length $t^{-\nu}$ is due to finite-size effects. The insert shows the oscillations of the rescaled boundary magnetization for different values of r after subtraction of a constant amplitude.

where $\tilde{m}(t^{-\nu})$ is a log-periodic scaling function of its argument. We make use of this oscillating behaviour to obtain a more precise determination of the critical temperature (in the range 10^{-11} – 10^{-12}) and of the values of the bulk and surface exponents by plotting the rescaled magnetization $mt^{-\beta}$ as a function of $\ln t^{-\nu}$ as shown in figure 5 in the case of the first layer.

The values of μ_c and β_1 that we consider suitable are the ones which allow an oscillating behaviour for the widest interval in the variable $\ln t^{-\nu}$. A modification of the boundary exponent β_1 would change the average slope of the oscillating regime. This could be due to corrections to scaling, but, if such corrections really existed, they should cancel in this range of temperatures (in the oscillating regime, t goes to values as small as 10^{-9}). The other parameters, μ_c , modifies the number of oscillations and we have chosen a value leading to the largest number of such oscillations. A poor determination of the critical point $\mu'_c = \mu_c + \Delta\mu_c$ would indeed artificially introduce a correction to scaling term, since $t^\beta = (t' + \Delta\mu_c)^\beta \sim t'^\beta (1 + \beta \frac{\Delta\mu_c}{t'})$.

The corresponding values of θ_c , β_1 and $\beta_{(n-1)}$ are given for several values of the perturbation amplitude r in table 2. The critical exponent associated to the right surface (m_L) of the Fibonacci chain has also been computed for different values of r for the largest chain size. It gives, with a good accuracy, the same value as for the left surface (m_1) as it can be seen by inspection in the table. The aperiodic sequence is indeed the same, seen from both ends, if we forget the last two digits.

Furthermore, the profiles of figure 3 clearly show that the sites of the chain are not all equivalent and the magnetization profiles can be locally rescaled with different values of the exponents depending on the site [18]. Thus, after the local quantities, the computation of the surface and mean bulk magnetizations enable us to determine the critical exponents respectively written as β_s and β_b and given in table 2.

From our values, one obviously recovers the usual unperturbed ordinary transition values of the exponents when the perturbation amplitude goes to zero.

Table 2. Numerical values of the critical temperature and the magnetic exponents for the surface and bulk magnetizations. The figure in parentheses gives the uncertainty on the last digit.

| r | θ_c | Surface | | | Bulk | |
|-----|-------------------------|--------------|------------|------------|-----------------|------------|
| | | β_1 | β_L | β_s | $\beta_{(n-1)}$ | β_b |
| 0.1 | 0.963 977 634 341 (5) | 1.000 36 (2) | — | 0.0002 (2) | 0.500 087 (1) | 0.5002 (2) |
| 0.2 | 0.931 876 799 29 (2) | 1.001 46 (2) | 1.0015 (1) | — | 0.500 33 (1) | — |
| 0.3 | 0.903 145 033 63 (2) | 1.003 4 (1) | 1.0034 (1) | — | 0.500 72 (6) | — |
| 0.5 | 0.854 041 490 87 (2) | 1.009 2 (1) | — | 0.0094 (2) | 0.501 87 (1) | 0.505 (1) |
| 0.8 | 0.796 437 160 887 (5) | 1.022 14 (2) | — | 0.0216 (2) | 0.504 19 (2) | — |
| 1.0 | 0.766 005 950 95 (2) | 1.032 7 (1) | — | 0.0302 (2) | 0.505 777 (2) | 0.516 (1) |
| 1.5 | 0.709 022 416 01 (2) | 1.062 1 (1) | — | — | 0.509 43 (1) | — |
| 2.0 | 0.670 109 092 37 (2) | 1.091 3 (1) | — | 0.087 (1) | 0.511 86 (3) | 0.538 (1) |
| 2.5 | 0.642 346 292 79 (2) | 1.117 8 (1) | — | — | 0.512 94 (1) | — |
| 3.0 | 0.621 796 760 462 (5) | 1.141 0 (1) | 1.1410 (1) | 0.133 (1) | 0.513 2 (1) | 0.555 (1) |
| 3.5 | 0.606 105 675 08 (2) | 1.160 2 (1) | — | — | 0.513 27 (4) | — |
| 4.0 | 0.593 804 120 472 (5) | 1.176 6 (1) | — | 0.1692 (4) | 0.513 0 (1) | 0.563 (1) |
| 4.5 | 0.583 941 173 69 (2) | 1.190 4 (1) | — | — | 0.512 2 (1) | — |
| 5.0 | 0.575 880 529 524 8 (5) | 1.202 6 (1) | — | 0.195 (1) | 0.511 25 (2) | 0.567 (1) |

3.3. Susceptibility and critical isotherm

Taking account of a non-vanishing bulk magnetic field in equations (6) and (7), one can compute the magnetization in a finite field and then deduce the critical isotherms exponents $\delta_{(n-1)}$ and δ_1 from the behaviour of the local magnetizations $m_{(n-1)}$ and m_1 with respect to h

$$m_{(n-1)} \sim h^{1/\delta_{(n-1)}} \quad m_1 \sim h^{1/\delta_1} \quad t = 0. \quad (27)$$

This time, a direct log–log plot allows a precise determination of the exponents and the rescaled equation of state confirms the validity of the estimate since we obtain a good data collapse. In the case of the boundary magnetization, the scaling assumption takes the following form under rescaling by an arbitrary factor b

$$m_1(t, h) = b^{-\beta_1/\nu} m_1(b^{y_t} t, b^{y_h} h) \quad (28)$$

where y_t is given by the inverse of the correlation length exponent $y_t = 1/\nu$ and the value of the magnetic field anomalous dimension y_h follows the requirements of (27): $y_h = \beta_1 \delta_1 / \nu = \beta \delta / \nu$. The choice $b = t^{-\nu}$ for the rescaling factor then leads to a universal behaviour expressed in terms of a single scaled variable

$$m_1(t, h) = t^{\beta_1} f_{m_1}^{\pm}(ht^{-\Delta}) \quad (29)$$

where $\Delta = \beta_1 \delta_1$ is the so-called gap exponent, $f_{m_1}^{\pm}$ is a universal scaling function and \pm refers to the two phases $\theta > \theta_c$ and $\theta < \theta_c$. This may then be checked by a plot of $m_1 t^{-\beta_1}$ versus $ht^{-\Delta}$ shown in figure 6 and the same type of universal functions have been obtained for the local bulk site $m_{(n-1)} t^{-\beta_{(n-1)}} = f_{m_{(n-1)}}^{\pm}(ht^{-\Delta})$. The values of δ_1 and $\delta_{(n-1)}$ are given in table 3.

The behaviours of m_s and m_b with h at the critical point lead to the values of δ_s and δ_b , also listed in table 3. We can point out the low accuracy in the determination of δ_s since the slope of the log–log plot of m_s versus h is quite small when r reaches the unperturbed value $r = 0$.

The derivative of equation (28) with respect to the bulk magnetic field h defines the boundary susceptibility χ_1 which diverges as the critical point is approached with an

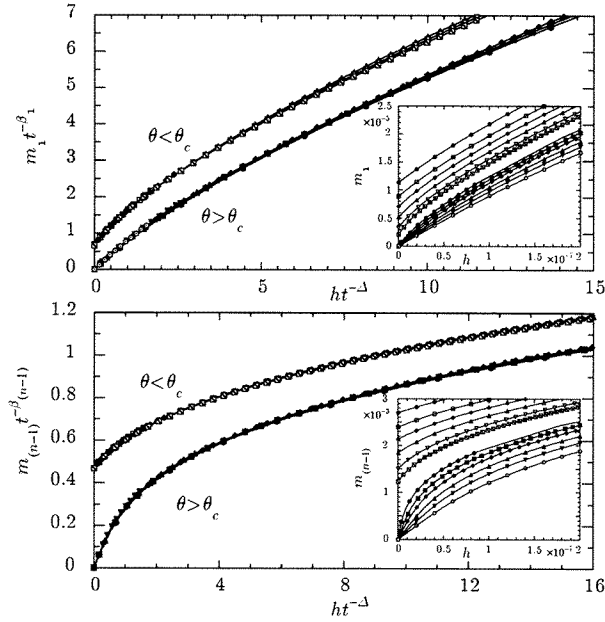


Figure 6. Rescaled equations of state for the boundary and bulk magnetization for $r = 2$. The values of the temperature are $\theta = 0.670\,090, 0.670\,094, 0.670\,097, 0.670\,100, 0.670\,103, 0.670\,105$ below θ_c and $0.670\,111, 0.670\,113, 0.670\,115, 0.670\,118, 0.670\,121, 0.670\,125$ above θ_c . Top: scaling functions $f_{m_1}^\pm$, the insert shows the boundary magnetization as a function of the bulk magnetic field. Bottom: same as above for the local bulk magnetization.

Table 3. Numerical values of the critical exponents associated to the critical isotherms and the susceptibilities. γ_b and δ_b correspond to the behaviour of the mean bulk magnetization m_b . The figure in parentheses gives the uncertainty on the last digit.

| r | Surface | | | | Bulk | | | |
|-----|------------|------------|------------|------------|------------------|------------------|-------------|-------------|
| | γ_1 | δ_1 | γ_s | δ_s | $\gamma_{(n-1)}$ | $\delta_{(n-1)}$ | γ_b | δ_b |
| 0.1 | 0.5013 (2) | 1.5024 (2) | 1.498 (1) | — | 0.9997 (1) | 2.9989 (1) | 1.0005 (1) | — |
| 0.2 | 0.5006 (2) | 1.5004 (2) | — | — | 0.9993 (2) | 2.9972 (3) | — | — |
| 0.3 | 0.4992 (2) | 1.4977 (2) | — | — | 0.9993 (2) | 2.9949 (9) | — | — |
| 0.5 | 0.4958 (2) | 1.4901 (2) | 1.493 (1) | 312 (11) | 0.9989 (2) | 2.9895 (9) | 0.99790 (2) | 2.98136 (2) |
| 0.8 | 0.487 (1) | 1.4751 (3) | 1.486 (1) | 85 (2) | 0.9986 (3) | 2.981 (2) | — | — |
| 1.0 | 0.4796 (2) | 1.4641 (2) | 1.480 (2) | 53 (1) | 0.9985 (4) | 2.9744 (9) | 0.99253 (2) | 2.93144 (2) |
| 1.5 | 0.4568 (2) | 1.4378 (4) | — | — | 0.9988 (7) | 2.963 (3) | — | — |
| 2.0 | 0.4316 (2) | 1.4135 (1) | 1.438 (2) | 16.37 (2) | 0.999 (2) | 2.9571 (1) | 0.9792 (1) | 2.82375 (3) |
| 2.5 | 0.412 (1) | 1.3845 (6) | — | — | 0.9992 (9) | 2.954 (2) | — | — |
| 3.0 | 0.388 (1) | 1.3484 (6) | 1.394 (2) | 11.2 (2) | 0.9988 (6) | 2.952 (2) | 0.9660 (1) | 2.7513 (2) |
| 3.5 | 0.372 (1) | 1.3108 (5) | — | — | 0.9986 (5) | 2.949 (2) | — | — |
| 4.0 | 0.354 (1) | 1.2989 (4) | 1.360 (2) | 10.01 (5) | 0.9988 (8) | 2.948 (2) | 0.9619 (5) | 2.6976 (3) |
| 4.5 | 0.341 (1) | 1.2571 (2) | — | — | 0.999 (1) | 2.950 (2) | — | — |
| 5.0 | 0.328 (1) | 1.2467 (6) | 1.330 (2) | 8.3 (4) | 0.999 (2) | 2.953 (2) | 0.9514 (2) | 2.65938 (2) |

exponent γ_1 . Numerically, the boundary magnetization is calculated for several values of the bulk magnetic field (of the order of 10^{-9}), and χ_1 follows a finite difference derivation. The bulk local susceptibility $\chi_{(n-1)}$ may be obtained in the same way. Log-

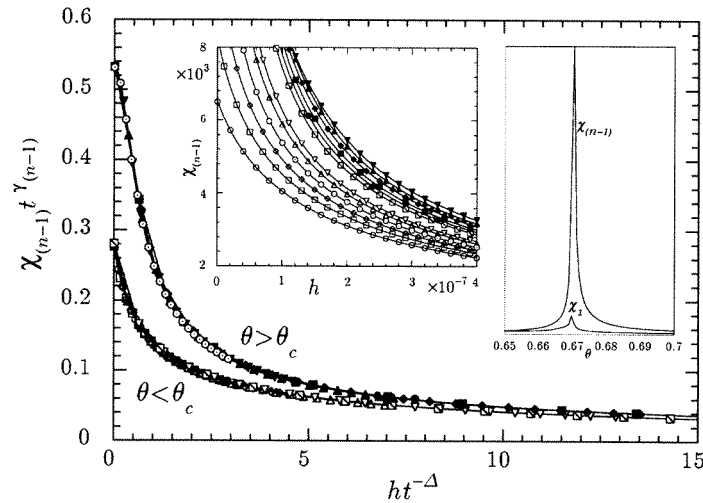


Figure 7. Rescaled bulk susceptibility giving the behaviour of the universal functions $f_{\chi_{(n-1)}}^{\pm}$ below and above θ_c for $r = 2$. The values of the temperature are the same as in figure 6. The inserts show the behaviours of $\chi_{(n-1)}$ as a function of h for the same temperatures (left), and the singularities of both $\chi_{(n-1)}$ and χ_1 in zero magnetic field as a function of θ (right).

periodic oscillations also occur in these quantities and the determination of the exponents can be done in the same way as in the previous section for the magnetization. Again, the accuracy of the result is confirmed by the rescaled curves for the susceptibilities, for example $\chi_{(n-1)} t^{\gamma_{(n-1)}} = f_{\chi_{(n-1)}}^{\pm}(ht^{-\Delta})$ shown in figure 7 exhibits a good data collapse on two universal curves for $\theta < \theta_c$ and $\theta > \theta_c$.

The values of the exponents are given in table 3 which presents also γ_s and γ_b , associated to the surface and average bulk magnetization field derivatives.

4. Specific heat

According to the definitions in section 2, the surface and bulk free energies are also defined as follows

$$F_s = \frac{1}{2}(F_{\text{FBC}} - F_{\text{PBC}}) \quad (30a)$$

$$F_b = F_{\text{PBC}} \quad (30b)$$

where F_{FBC} and F_{PBC} denote the total free energies of aperiodic chains with free and periodic boundary conditions respectively and are obtained numerically using equations (19) and (20).

The expected singular behaviours of the free energy densities

$$f_s(t, h) = t^{2-\alpha_s} f_s(ht^{-\Delta}) \quad (31a)$$

$$f_b(t, h) = t^{2-\alpha_b} f_b(ht^{-\Delta}) \quad (31b)$$

where the dependence of f_s with the local magnetic surface field h_1 has been omitted since we always consider the case $h_1 = 0$, lead to the surface and bulk specific heat exponents. The values of α_s and α_b are simply deduced from the slopes of the log-log plots of f_s and f_b versus t .

In figure 8, we show the bulk free energy density amplitude $f_b t^{\alpha_b - 2}$ as a function of $\ln t^{-\nu}$ for $r = 2$. It exhibits the same type of oscillating behaviour than the rescaled magnetization of figure 5.

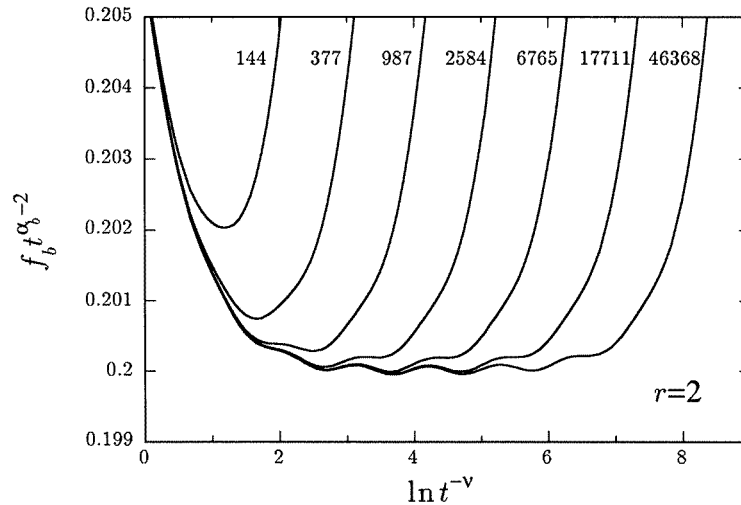


Figure 8. Rescaled bulk free energy density $f_b t^{\alpha_b - 2}$ versus $\ln t^{-\nu}$ for $r = 2$. The amplitude of the bulk free energy density exhibits log-periodic oscillations.

Table 4. Numerical values of the specific heat critical exponents. The figure in parentheses gives the uncertainty on the last digit.

| r | α_s | α_b |
|-----|--------------|---------------|
| 0.1 | 0.514 96 (7) | -0.000 31 (1) |
| 0.5 | 0.501 12 (5) | -0.007 33 (1) |
| 0.8 | 0.484 48 (5) | -0.017 09 (1) |
| 1.0 | 0.470 75 (4) | -0.024 62 (1) |
| 2.0 | 0.402 65 (1) | -0.059 24 (1) |
| 3.0 | 0.350 77 (4) | -0.078 13 (1) |
| 4.0 | 0.315 16 (3) | -0.085 79 (1) |
| 5.0 | 0.289 35 (6) | -0.088 05 (1) |

The surface and bulk specific heat exponents are collected in table 4. The bulk specific heat discontinuity of the homogeneous system is washed out in the perturbed system, since $\alpha_b < 0$.

5. Discussion

We have numerically calculated several surface and bulk critical exponents for a marginal aperiodic system within mean field theory. The marginal aperiodicity leads to exponents which vary continuously with the amplitude of the perturbation r . The variations of these exponents are shown in figure 9 as a function of r .

The comparison in table 2 between the bulk exponent β_b and the local one $\beta_{(n-1)}$ clearly shows that it is no longer possible, in this aperiodic system, to define a unique bulk exponent, as it was already suggested by the possibility of a local rescaling of the profiles with position-dependent exponents which suggests a multiscaling behaviour. A constant value $\gamma_1 = 1/\nu$ is consistent with continuously varying exponents, in order to keep a vanishing crossover exponent which ensures that the marginality condition remains

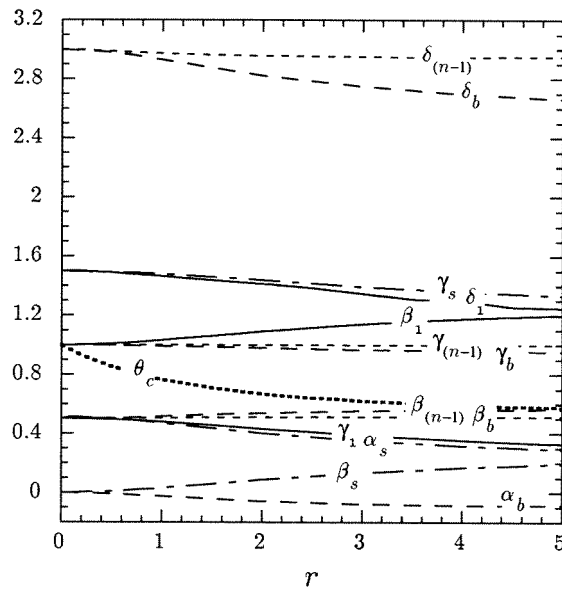


Figure 9. Variations of the surface and bulk exponents with the perturbation amplitude r (boundary exponents: —, surface: — · —, local bulk: - - -, mean bulk: — — —).

valid for any value of the aperiodicity amplitude r . On the other hand, for y_h there is no such reason. From this point of view, equations like (28) are not exact since a unique field anomalous dimension y_h has no real significance. It follows that the universal functions in figures 6 and 7 only give an approximate picture of the scaling behaviour in this system, since they involve the gap exponent $\Delta = y_h/y_t$. The good data collapse has to be credited to the weak variation of the exponents with the perturbation amplitude r .

On the other hand, the scaling laws involving the dimension of the system are satisfied in mean field theory with a value of d equal to the upper critical dimension d^* . As for the $2d$ Ising model with a marginal aperiodicity [17, 18], one expects a strongly anisotropic behaviour in the Gaussian model. It yields a continuous shift of the upper critical dimension with the perturbation amplitude, $d^*(r)$, since the value $d^* = 4$ for a critical point in the homogeneous ϕ^4 theory follows Ginzburg's criterion for an isotropic behaviour. Hyperscaling relations should thus be satisfied for the mean field exponents with $d^*(r)$

$$2 - \alpha_b = \nu d^*(r) \quad (32a)$$

$$2 - \alpha_s = \nu(d^*(r) - 1). \quad (32b)$$

We can make use of these relations to obtain an estimate of the upper critical dimension $d^*(r)$ for this aperiodic system. The corresponding results are given in table 5.

The two determinations are in good agreement for small values of the perturbation amplitude. The discrepancy at larger values of r suggests that the precision in the determination of the exponents has probably been overestimated, but the variation of the upper critical dimension with the perturbation amplitude is clear and should be attributed to an anisotropic scaling behaviour in the corresponding Gaussian model.

One can finally mention that a mean field approach for relevant aperiodic perturbations would be interesting. Many cases of aperiodic sequences with a wandering exponent

Table 5. Numerical values of the upper critical dimension $d^*(r)$ deduced from hyperscaling relations.

| r | $(2 - \alpha_b)/\nu$ | $(2 - \alpha_s)/\nu + 1$ |
|-----|----------------------|--------------------------|
| 0.1 | 4.00 | 3.97 |
| 0.5 | 4.01 | 4.00 |
| 0.8 | 4.03 | 4.03 |
| 1.0 | 4.05 | 4.06 |
| 2.0 | 4.12 | 4.19 |
| 3.0 | 4.16 | 4.28 |
| 4.0 | 4.17 | 4.37 |
| 5.0 | 4.18 | 4.42 |

$\omega > -1$ are known, they constitute relevant perturbations in mean field theory. In the case of the $2d$ layered Ising model with relevant perturbations, a behaviour which looks like random systems behaviour, with essential singularities, was found [16], and the same type of situation can be expected within mean field approximation.

Acknowledgments

We thank L Turban for valuable discussions and F Iglói and G Palàgyi for informing us of a related work before publication. This work has been supported by the Groupe CNI/Matière under project CNI1155C96.

References

- [1] Schechtman D, Blech I, Gratias D and Cahn J W 1984 *Phys. Rev. Lett.* **53** 1951
- [2] Henley C L 1987 *Comment. Condens. Matter Phys.* **13** 59
Janssen T 1988 *Phys. Rep.* **168** 55
Janot C, Dubois J M and de Boissieu M 1989 *Am. J. Phys.* **57** 972
Guyot P, Kramer P and de Boissieu M 1991 *Rep. Prog. Phys.* **54** 1373
Steinhardt P and DiVicenzo D 1991 *Quasicrystals: The State of the Art* ed P Steinhardt and D DiVicenzo (Singapore: World Scientific)
- [3] Grimm U and Baake M 1996 *Preprint* cond-mat/9604116
- [4] Majkrzak C F, Kwo J, Hong M, Yafet Y, Gibbs D, Chien C L and Bohr J 1991 *Adv. Phys.* **40** 99
- [5] Ginzburg V L and Landau L D 1965 *Collected Papers of L D Landau* ed D Ter Haar (New York: Gordon and Breach) p 546
Ginzburg V L and Pitaevskii L P 1958 *Sov. Phys.-JETP* **34** 858
- [6] Mills D L 1971 *Phys. Rev. B* **3** 3887
Kaganov M I and Omel' Yanchuk A N 1972 *Sov. Phys.-JETP* **34** 895
Kagonov M I 1972 *Sov. Phys.-JETP* **35** 631
Binder K and Hohenberg P C 1972 *Phys. Rev. B* **6** 3461
Barber M N 1973 *Phys. Rev. B* **8** 407
Kumar P 1974 *Phys. Rev. B* **10** 2928
Lubensky T C and Rubin M H 1975 *Phys. Rev. B* **12** 3885
- [7] Bray A J and Moore M A 1977 *J. Phys. A: Math. Gen.* **10** 1927
Fisher M E 1973 *J. Vac. Sci. Technol.* **10** 665
Bray A J and Moore M A 1977 *Phys. Rev. Lett.* **38** 1046
Diehl H W and Dietrich S 1981 *Z. Phys. B* **42** 65
Diehl H W 1982 *J. Appl. Phys.* **53** 7914
Diehl H W and Dietrich S 1981 *Z. Phys. B* **42** 65
- [8] Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (London: Academic) p 1

- [9] Luck J M 1993 *J. Stat. Phys.* **72** 417
- [10] Luck J M 1993 *Europhys. Lett.* **24** 359
Iglói F 1993 *J. Phys. A: Math. Gen.* **26** L703
- [11] Harris A B 1974 *J. Phys. C: Solid State Phys.* **7** 1671
- [12] Queffelec M 1987 *Substitution Dynamical Systems (Lecture Notes in Mathematics 1294)* ed A Dold and B Eckmann (Berlin: Springer) p 97
Dumont J M 1990 *Number Theory and Physics (Springer Proceedings in Physics 47)* ed J M Luck, P Moussa and M Waldschmidt (Berlin: Springer) p 185
- [13] Iglói F 1988 *J. Phys. A: Math. Gen.* **21** L911
Doria M M and Satija I I 1988 *Phys. Rev. Lett.* **60** 444
Tracy C A 1988 *J. Stat. Phys.* **51** 481
Tracy C A 1988 *J. Phys. A: Math. Gen.* **21** L603
Benza G V 1989 *Europhys. Lett.* **8** 321
Ceccatto H A 1989 *Phys. Rev. Lett.* **62** 203
Ceccatto H A 1989 *Z. Phys. B* **75** 253
Henkel M and Patkós A 1992 *J. Phys. A: Math. Gen.* **25** 5223
- [14] Doria M M, Nori F and Satija I I 1989 *Phys. Rev. B* **39** 6802
Lin Z and Tao R 1990 *Phys. Lett. A* **150** 11
- [15] Lin Z and Tao R 1992 *J. Phys. A: Math. Gen.* **25** 2483
Lin Z and Tao R 1992 *Phys. Rev. B* **46** 10 808
You J Q, Yan J R and Zhong J X 1992 *J. Math. Phys.* **33** 3901
Turban L and Berche B 1993 *Z. Phys. B* **92** 307
Turban L, Iglói F and Berche B 1994 *Phys. Rev. B* **49** 12 695
Turban L, Berche P E and Berche B 1994 *J. Phys. A: Math. Gen.* **27** 6349
Iglói F, Lajkó P and Szalma F 1995 *Phys. Rev. B* **52** 7159
Iglói F and Turban L 1996 *Phys. Rev. Lett.* **77** 1206
- [16] Iglói F and Turban L 1994 *Europhys. Lett.* **27** 91
- [17] Berche B, Berche P E, Henkel M, Iglói F, Lajkó P, Morgan S and Turban L 1995 *J. Phys. A: Math. Gen.* **28** L165
Iglói F and Lajkó P 1996 *J. Phys. A: Math. Gen.* **29** 4803
- [18] Berche P E, Berche B and Turban L 1996 *J. Physique* **6** 621
- [19] Karevski D, Palágyi G and Turban L 1995 *J. Phys. A: Math. Gen.* **28** 45
- [20] Grimm U and Baake M 1994 *J. Stat. Phys.* **74** 1233
Karevski D, Turban L and Iglói F 1995 *J. Phys. A: Math. Gen.* **28** 3925
- [21] Landau L D 1937 *Collected Papers of L D Landau* ed D Ter Haar (New York: Gordon and Breach) p 193
- [22] Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (London: Academic) p 146
- [23] Jona-Lasinio G 1975 *Nuovo Cimento* **26B** 99
Nauenberg M 1975 *J. Phys. A: Math. Gen.* **8** 925
Niemeijer T and van Leeuwen J M J 1976 *Phase Transitions and Critical Phenomena* vol 6, ed C Domb and M S Green (London: Academic) p 425
Karevski D and Turban L 1996 *J. Phys. A: Math. Gen.* **29** 3461