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Surface magnetization and surface correlations in aperiodic Ising models

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Abstract. We consider the surface critical behaviour of diagonally layered Ising models on the square lattice where the inter-layer couplings follow some aperiodic sequence. The surface magnetization is analytically evaluated from a simple formula derived by the diagonal transfer matrix method, while the surface spin–spin correlations are obtained numerically by a recursion method, based on the star–triangle transformation. The surface critical behaviour of different aperiodic Ising models is found in accordance with the corresponding relevance–irrelevance criterion. For marginal sequences the critical exponents are continuously varying with the strength of aperiodicity and generally the systems follow anisotropic scaling at the critical point.

1. Introduction

The discovery of quasi-crystals [1] has stimulated intensive research to understand their structure and physical properties (for recent reviews see [2–6]). Theoretically a challenging problem is to determine the critical properties of such quasiperiodic or more generally aperiodic structures. After a series of numerical [7–13] and analytical [14–21] studies on specific models Luck has proposed a relevance–irrelevance criterion [22]. According to this criterion, which is a generalization of the Harris criterion for random magnets [23], the inhomogeneity is irrelevant (relevant) if the fluctuating energy in the scale of the bulk correlation length is smaller (greater) than the excess thermal energy. In layered systems the above criterion is connected to the sign of the cross-over exponent

$$\phi = 1 + \nu(\omega - 1) \tag{1}$$

which is expressed in terms of the correlation length exponent ν of the unperturbed system and the wandering exponent of the sequence ω [24].

Most of the studies about the critical properties of aperiodic systems are restricted to the quantum Ising chain with aperiodic couplings [22, 25–34], which is equivalent to the twodimensional classical, layered Ising model in the extreme anisotropic limit [35]. According to (1) for this model with $\nu = 1$ sequences with bounded (unbounded) fluctuations represent irrelevant (relevant) perturbations. The analytical and numerical results obtained on different physical quantities (specific heat, surface and bulk magnetization, local energy density, etc) of different aperiodic Ising quantum chains are consistent with the prediction of the Luck criterion. For marginal sequences non-universal critical behaviour was found [30, 31], even if the aperiodic perturbation was of radial symmetry [34]. We note also some related studies on hierarchical Ising models [36].

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In the present paper we study the surface magnetization and the surface spin-spin correlations of aperiodic Ising models. In contrast to previous investigations we consider here the classical version of the model with a layered aperiodicity in the diagonal direction and the critical properties are studied on the (1, 1) surface of a square lattice. We use two methods of investigation. The surface magnetization is calculated analytically with the diagonal transfer matrix method [37–39], whereas both the surface magnetization and surface correlations are numerically studied by a recursion method based on the star-triangle transformation. This latter method has also been used to study layered triangular systems. We note that some preliminary results of our investigations have already been announced in a letter [30].

The structure of the paper is the following. In sections 2 and 3 we present the diagonal transfer matrix method and the star-triangle recursion method, respectively. Results on different aperiodic Ising models are given in section 4. A discussion is contained in section 5, while details of the calculation are presented in the appendix.

2. Surface magnetization by the transfer matrix method

Let us consider an Ising model on the square lattice with a diagonally layered structure, where the nearest neighbour couplings in the *i*th layer from the surface are given by $J_i = K_i k_B T$ (see figure 1(*a*)). We are interested in the magnetization at the (1, 1) surface, which is calculated in the transfer matrix formalism [37–39]. Denoting by $\langle 0 |$ and $\langle 1 |$ the ground state and the first excited state of the T diagonal transfer matrix, respectively, the surface magnetization is given by the matrix element of the surface spin-flip operator σ_1^x ,

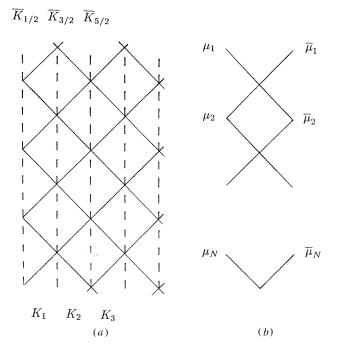


Figure 1. (*a*) Diagonally layered square lattice (full line) and the corresponding triangular lattice with broken vertical lines. For the square lattice the vertical couplings are zero $\overline{K}_i = 0$. (*b*) Portion of the lattice contained in the square of the diagonal transfer matrix.

as

$$m_s = \langle 0 | \sigma_1^x | 1 \rangle.$$

Working with free boundary conditions T is different in odd and even sites, therefore we consider T^2 , which is given for the inhomogeneous model as

$$(\mathbf{T}^{2})_{\mu,\overline{\mu}} = 2^{N} \prod_{i=1}^{N-1} \cosh[K_{2i-1}(\mu_{i} + \overline{\mu}_{i}) + K_{2i}(\mu_{i+1} + \overline{\mu}_{i+1})] \cosh[K_{2N-1}(\mu_{N} + \overline{\mu}_{N})]$$
(2)

and depends on the configurations of the $\mu_i = \pm 1$ and $\overline{\mu}_i \pm 1$ spins, i = 1, 2, ..., N (figure 1(*b*)).

To determine the eigenvectors of T^2 we make use of the fact that T^2 and the linear operator

$$H = -\sum_{i=1}^{N-1} \lambda_i \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^N h_i \sigma_i^x$$
(3)

commute:

$$[\boldsymbol{T}^2, \boldsymbol{H}] = 0 \tag{4a}$$

if the couplings of the inhomogeneous quantum Ising chain in (3) satisfy the relations

$$h_i \frac{C_{2i-2}}{C_{2i}} = h_{i+1} \frac{C_{2i+1}}{C_{2i-1}} \tag{4b}$$

and

$$\lambda_i = h_i S_{2i} S_{2i-1} \frac{C_{2i-2}}{C_{2i}}.$$
(4c)

Here we used the abbreviations $\sinh 2K_i \equiv S_i$, $\cosh 2K_i \equiv C_i$ and $C_0 = 1$. Derivation of (4a-c) is shown in the appendix. According to (4a) the eigenvectors of T^2 and H are the same, therefore we evaluate the matrix element of the surface of magnetization $\langle 0|\sigma_1^x|1\rangle$ for the inhomogeneous quantum Ising chain. Using a free fermionic representation of H [40] one can show [41] that

$$m_s = \Phi_s(1) \tag{5}$$

and the Φ_s vector is determined by the equation $(A + B)\Phi_s = 0$, where

From the normalization condition $\sum_{i} \Phi_s^2(i) = 1$ one obtains for the surface magnetization

$$m_s = \left[1 + \sum_{i=1}^{\infty} \prod_{j=1}^{i} \left(\frac{h_j}{\lambda_j}\right)^2\right]^{-1/2} = \left[1 + \sum_{i=1}^{\infty} \prod_{j=1}^{i} S_j^{-2}\right]^{-1/2}$$
(7)

where in the last equation we have used (4*b*) and (4*c*). Analysing the formula in (7) we can say that the magnetization on the (1, 1) surface of a diagonally layered Ising model is formally the same as that of a quantum Ising chain with inhomogeneous couplings $\lambda_i = \sinh 2K_i$ and in uniform transverse field $h_i = 1$ [41]. We note that for the homogeneous Ising model (7) gives Peschel's result [42]: $m_s = (1 - \sinh^{-2} 2K)^{-1/2}$.

3. Recursion method

The Ising model on the triangular lattice is invariant under the star-triangle transformation [43] (STT), which makes the exact solution of the model on this lattice relatively simple [44]. Also, an exact renormalization group transformation for the triangular Ising model is based on the repeated use of the STT [45]. For a semi-infinite Ising model the STT has been used by Hilhorst and van Leeuwen [46] and by others [47,48] to construct an iterative procedure to calculate the surface magnetization and the surface correlations in the triangular Ising model. The method can be succesfully used for layered systems in which the couplings are the same within one layer. We note that the square lattice can be considered as a special case of the triangular lattice with vanishing couplings across the diagonals (figure 1(a)). In the following we briefly recapitulate the basic results of the recursion method.

Let us consider a layered Ising model on a semi-infinite triangular lattice with vertical couplings parallel to the surface \overline{K}_i , $i = \frac{1}{2}, \frac{3}{2}, \ldots$ and with diagonal couplings K_i , $i = 1, 2, \ldots$ (figure 1(*a*)). The STT maps the triangular lattice onto a hexagonal lattice which is in turn equivalent to a new triangular lattice. Iterating this mapping a sequence of triangular Ising models is generated ($n = 0, 1, 2, \ldots$) with couplings $\overline{K}_i(n)$ and $K_i(n)$ from the original model with n = 0. The surface magnetization $m_s(n)$ and the surface spin-spin correlation function $g_s(l, n) = \langle \sigma_{1,l}\sigma_{1,0} \rangle - \langle \sigma_1 \rangle^2$ transform as [46]

$$m_{s}(n) = \{1 - \exp[-4\overline{K}_{1/2}(n+1)]\}^{1/2}m_{s}(n+1)$$

$$g_{s}(l,n) = \frac{1}{4}\{1 - \exp[-4\overline{K}_{1/2}(n+1)]\}[g_{s}(l+1,n+1)]$$
(8a)

$$+2g_{s}(l, n+1) + g_{s}(l-1, n+1)].$$
(8b)

Making use of the boundary condition $g_s(0, n) = 1 - m_s^2(n)$ one obtains for the original model with $m_s = m_s(0)$ and $g_s(l) = g_s(l, 0)$ [46]

$$m_{s} = \lim_{n \to \infty} [f(n)]^{1/2} m_{s}(n)$$

$$g(l) = \sum_{n=1}^{\infty} 4^{-n} \frac{l}{n} {2n \choose n+l} f(n) [1 - m_{s}^{2}(n)]$$

$$f(n) = \prod_{j=1}^{n} \{1 - \exp[-4\overline{K}_{1/2}(n+1)]\}.$$
(9)

These relations are exact and can be used to iterate on a computer for any type of distribution of the couplings in the original layered model. In this way calculating the surface magnetization one can numerically determine the T_c critical point and the β_s critical exponent of the surface magnetization of the model from $m_s(t) \sim t^{\beta_s}$ as $t = (T_c - T)/T_c \rightarrow 0$. For the square lattice with $\overline{K}_i(0) = 0$ these results should be compared with the analytical expression in (7).

To obtain analytical results by the recursion method one should analyse the asymptotic behaviour of $X(n) = \exp[-4\overline{K}_{1/2}(n)]$, since according to numerical observations X(n) is smoothly varying with $n \gg 1$ [48]. Inserting the asymptotic solution of X(n) into (9) one obtains in the continuum approximation:

$$m_s = [f(n_0)]^{1/2} \exp\left[-\frac{1}{2} \int_{n_0}^{\infty} X(n) \,\mathrm{d}n\right]$$
(10)

and

$$g_s(l) = \sum_{n=l}^{\infty} \frac{l}{n^{3/2}} \frac{1}{\sqrt{n}} \exp(-l^2/n) [f(n) - f(\infty)]$$
(11)

where n_0 is a finite cut-off, on which the critical exponents do not depend. According to (10) the surface magnetization is non-zero if the integral $\int_{n_0}^{\infty} X(n) dn$ is convergent, thus X(n) goes to zero faster than 1/n, as *n* tends to infinity.

The asymptotic behaviour of X(n) has been calculated exactly at the critical point of the homogeneous model and for models with smoothly varying couplings at the surface [46–48], but there are no exact results available on X(n) outside the critical point. For the homogeneous, critical Ising model [46] $X(n) \simeq 1/2n$, thus $m_s(t = 0) = 0$, $f(n) \sim n^{-1/2}$ and the surface correlations from (11) decay as $g_s(l) \sim l^{-\eta_{\parallel}}$ with $\eta_{\parallel} = 1$. For general inhomogeneous models the decay exponent follows from the asymptotic behaviour:

$$\lim_{n \to \infty} 2nX(n) = \eta_{\parallel}.$$
(12)

In numerical calculations it is more accurate to determine the decay exponent from (12), than to investigate the magnetization exponent β_s from the behaviour of the surface magnetization outside the critical point.

4. Results on aperiodic models

Although one can study general, triangular Ising models by the recursion method, here we restrict ourselves to the (1, 1) surface of diagonally layered square models. In this way we reduce the space of parameters with $\overline{K}_i = 0$; furthermore we make use of the analytical expression on the surface magnetization in (7).

The criticality condition for layered inhomogeneous Ising models [49] is expressed in terms of the variable $S_i = \sinh 2K_i$ as

$$\lim_{L \to \infty} \frac{1}{L} \sum_{i=1}^{L} \log S_i = 0.$$
(13)

Here we study two-valued sequences of the couplings and use the parametrization $S_i = Sr^{f_i}$, where f_i takes the values 0 or 1 according to an aperiodic sequence. The homogeneous model is described by r = 1. The fluctuation of the couplings in a domain of size L is characterized by the cumulated deviation from the average value \overline{S} as [50]

$$\Delta(S) = \sum_{i=1}^{L} (S_i - \overline{S}) \approx \delta L^{\omega} F\left(\frac{\ln L}{\ln \Lambda_1}\right).$$
(14)

Here $\delta = \overline{S}(r-1)$ is the amplitude of the modulation, ω is the wandering exponent, which is expressed by the leading eigenvalues of the substitutional matrix [24] $\omega = \ln |\Lambda_2| / \ln \Lambda_1$, and F(x) is a fractal function of its argument with period unity. From the transformation law of δ under scaling one can obtain the crossover exponent ϕ [25] in (1) and the corresponding relevance–irrelevance criterion as described in the introduction. The aperiodic sequences we consider in the following represent different types of perturbation according to this relevance–irrelevance criterion.

4.1. Irrelevant perturbation: Thue–Morse sequence

The binary Thue–Morse sequence [51] is generated through the substitution $0 \rightarrow 01$ and $1 \rightarrow 10$, so that one obtains after four steps:

This sequence represents an irrelevant perturbation, since $\Lambda_2 = 0$ and $\omega = -\infty$.

The surface magnetization can be obtained from (7) using the corresponding result for the Thue–Morse quantum Ising chain in [27]:

$$m_s = \frac{2t^{1/2}}{r^{1/2} + r^{-1/2}} \left[1 + \frac{1}{4} \left(\frac{r-1}{r+1} \right)^2 t + \mathcal{O}(t^2) \right]$$
(15)

where the critical point is at $S_c = r^{-1/2}$ and $t = 1 - (S_c/S)^2$. The surface magnetization exponent $\beta_s = \frac{1}{2}$ takes the value for homogeneous Ising systems. A similar conclusion can be obtained from a study of surface critical correlations. According to numerical results the relation in (12) $\lim_{n\to\infty} 2nX(n) = \eta_{\parallel} = 1$ is satisfied with an accuracy of 10^{-5} . Thus the decay exponent also takes the value for homogeneous Ising systems in two dimensions and the perturbation is indeed irrelevant as expected from scaling.

4.2. Relevant perturbation: Rudin–Shapiro sequence

The Rudin–Shapiro sequence [51] is generated by the two-digit substitution $00 \rightarrow 0001$, $01 \rightarrow 0010$, $10 \rightarrow 1101$ and $11 \rightarrow 1110$, thus one obtains after three substitutions:

The wandering exponent of the sequence is $\omega = \frac{1}{2}$, thus according to (1) this type of perturbation is relevant for the Ising model. The critical point from (13) is given by $S_c = r^{-1/2}$ as for the Thue–Morse model. The surface magnetization is again obtained from (7) using the known results about the corresponding Ising quantum chain in [28]. The surface magnetization behaves differently for r < 1 and r > 1. For r < 1, when the couplings at the surface are locally stronger than the average, the surface stays ordered at the critical point and the surface phase transition is of first order. The critical surface magnetization is given by [28]

$$m_{s,c} = \frac{1-r}{\sqrt{1-r+r^2}} \qquad r \leqslant 1.$$
 (16)

In the other regime, r > 1, the couplings are locally weaker at the surface than in the bulk and the surface magnetization behaves anomalously; it has an essential singularity at the critical point:

$$m_s \sim \exp[-\text{constant}(r-1)^2 t^{-1}]$$
 $r > 1.$ (17)

According to numerical results the decay of critical surface correlations is also anomalous. The quantity $\lim_{n\to\infty} 2nX(n) \to \infty$, thus according to (12) at the critical point the surface correlations decay faster than any power and $g_s(l)$ has a stretched exponential dependence on l.

4.3. Marginal perturbations

4.3.1. Fredholm sequence. The Fredholm sequence [51] is generated through substitution of the three letters A, B and C as $A \rightarrow AB$, $B \rightarrow BC$, $C \rightarrow CC$ and we associate $f_i = 0$ to the letters A and C and $f_i = 1$ to B. Starting with a letter A we get for the f_i series after four substitutions:

01101000100000000.

This type of perturbation is localized to the surface and there is no change in the critical temperature, thus $S_c = 1$. The sequence is marginal, since the corresponding wandering exponent $\omega = 0$. To evaluate the formula in (7) for the surface magnetization we use [33].

For $r > \sqrt{2}$ the surface transition is of first order, the critical surface magnetization is given by

$$m_{s,c} = \sqrt{\frac{r^2 - 2}{2r^2 - 3}} \qquad r \ge \sqrt{2}.$$
 (18)

In the other regime $r < \sqrt{2}$ the surface transition is of second order and the corresponding surface magnetization exponent is a continuous function of the parameter r:

$$\beta_s = \frac{1}{2} - \frac{\ln r}{\ln 2} \qquad r \leqslant \sqrt{2}. \tag{19}$$

Using the recursion method we have determined the decay exponent of suface correlations from (12), which is shown in figure 2 for $r \leq \sqrt{2}$. Comparing $\eta_{\parallel}(r)$ with the surface magnetization exponent $\beta_{s}(r)$ in (19) we can say that the surface scaling law [52]

$$\eta_{\parallel} = 2\beta_s/\nu \tag{20}$$

is satisfied for $r \leq \sqrt{2}$.

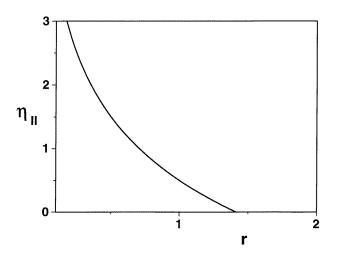


Figure 2. Decay exponent of critical surface spin-spin correlations for the Fredholm Ising model.

4.3.2. Period-doubling sequence. The period-doubling sequence follows from the substitution [51] $1 \rightarrow 10$ and $0 \rightarrow 11$, so that starting with a 1 after four steps we have

The critical temperature from (13) is $S_c = r^{-2/3}$; furthermore the sequence is marginal since $\omega = 0$. The critical exponent of the surface magnetization can be analytically determined using (7) and the corresponding result for the Ising quantum chain in [27]:

$$\beta_s = \frac{\ln[(1+r^{2/3})(1+r^{-2/3})]}{4\ln 2}.$$
(21)

As seen from equation (21), $\beta_s(r)$ is continuously varying with the parameter *r*. Furthermore it is the same at both ends of the chain. This is a consequence of the fact that omitting the last digit the period-doubling sequence is symmetric.

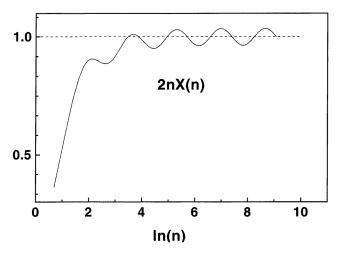


Figure 3. The quantity 2nX(n) as a function of the logarithm of the iterations for the perioddoubling Ising model with r = 2. The decay exponent $\eta_{\parallel} = 1$ in (12) is approached through log-periodic oscillations.

Next we calculate the decay exponent of critical correlations by the recursion method. In contrast to the surface magnetization exponent the decay exponent is found to be $\eta_{\parallel} = 1$, independently of the inhomogeneity parameter r. In figure 3 we show for r = 2 the quantity 2nX(n) as a function of the logarithm of the iterations. Its limiting value as $n \to \infty$ gives the decay exponent according to (12). The log-periodic oscillations for large n are a consequence of discrete scaling, which can be observed in other quantities as well (see (14)). We note that the same value of the decay exponent is found on the right boundary of the system.

Comparing the surface magnetization exponent in (21) and the decay exponent $\eta_{\parallel} = 1$ we can say that the surface scaling law in (20) does not satisfy. We shall come back to clear this point in section 5.

4.3.3. Paper-folding sequence. The paper-folding sequence [51] is obtained by recurrent folding of a sheet of paper, right over left. After unfolding one obtains a series of up- (1) and down-folds (0). The same sequence can be generated using the two-letter substitutions $00 \rightarrow 1000, 01 \rightarrow 1001, 10 \rightarrow 1100$ and $11 \rightarrow 1101$. Starting with 11 after three substitutions the sequence is given by

This sequence is also marginal, since $\omega = 0$; furthermore the critical point from (13) is $S_c = r^{-1/2}$.

Again the surface magnetization exponent is analytically known from (7) and using the result for the corresponding quantum Ising chain in [31]. At the left surface

$$\beta_s = \frac{\ln(1+r^{-1})}{2\ln 2} \tag{22}$$

whereas at the right boundary

$$\overline{\beta}_s = \frac{\ln(1+r)}{2\ln 2} \tag{23}$$

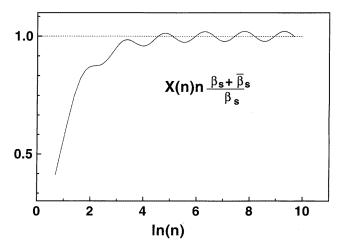


Figure 4. The quantity $nX(n)(\beta_s + \overline{\beta}_s)/\beta_s$ as a function of the logarithm of the iterations for the paper-folding Ising model with r = 2. The decay exponent $\eta_{\parallel} = (\beta_s + \overline{\beta}_s)/\beta_s$ in (12) is approached through log-periodic oscillations.

which is obtained by exchanging perturbed and unperturbed couplings, i.e. with $r \rightarrow r^{-1}$. Thus for the paper-folding sequence, which is not inversion symmetric, the surface magnetization exponents are different at the two boundaries.

Next we turn to calculate the decay exponent on the left boundary by the recursion method. Now η_{\parallel} is found *r*-dependent and for all *r* it satisfies the relation

$$\eta_{\parallel} = \frac{2\beta_s}{\beta_s + \overline{\beta}_s} \tag{24}$$

and a similar equation is true on the right surface with $\beta_s \leftrightarrow \overline{\beta}_s$. To illustrate the relation in (24) we show in figure 4 for r = 2 the quantity $nX(n)(\beta_s + \overline{\beta}_s)/\beta_s$, which tends to unity with log-periodic oscillations, in accordance with (12). We can say that the surface scaling law in (20) is again violated, like the period-doubling sequence.

5. Discussion

In this paper we have studied the surface magnetization and the surface correlation function of diagonally layered Ising models on the (1, 1) surface. For different aperiodic distributions of the diagonal couplings we have obtained exact results for the surface magnetization exponent by the diagonal transfer matrix method, whereas the decay of surface correlations was studied numerically by a recursion method based on the repeated use of the star-triangle transformation. The results obtained are in accord with the relevance-irrelevance criterion by Luck [22]. For the relevant Rudin–Shapiro model, first-order surface transition and anomalous decay of critical surface correlations were observed. For marginal sequences (Fredholm, period-doubling and paper-folding) non-universal surface critical behaviour was found, and the corresponding surface magnetization exponents continuously varied with the inhomogeneity parameter r.

The above observations remain valid, where the general triangular lattice Ising model with couplings K_i and \overline{K}_i is concerned. Then, besides the aperiodicity ratio r, another parameter \overline{K}_i/K_i enters the expressions. In this general case the criticality condition is also

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known analytically [49]:

$$\lim_{L \to \infty} \frac{1}{L} \sum_{i=1}^{L} \log S_i + 2\overline{K}_i = 0$$
⁽²⁵⁾

while both the surface magnetization and the surface correlations have to be calculated numerically by the recursion method. Our results on the triangular lattice qualitatively agree with that on the diagonal square lattice, and they satisfy the relevance–irrelevance criterion in (1) for all sequences. For marginal sequences continuously varying critical exponents were found, which depend on two parameters. Also the corresponding scaling relations are satisfied: equation (20) for the Fredholm sequence and equation (24) for the period-doubling and paper-folding sequences.

Finally, we come to the point of explaining the violation of surface scaling relation in (20) for the period-doubling and paper-folding sequences. The observed scaling behaviour in (24) is compatible with anisotropic scaling, when the correlation lengths parallel with ξ_{\parallel} and perpendicular to the surfaces ξ_{\perp} are diverging with different exponents, so that $\xi_{\parallel} \sim \xi_{\perp}^z$, where z is the anisotropy exponent. According to anisotropic scaling [53] the critical spin–spin correlation function on the left surface behaves as

$$g_s(l,t) = b^{-2\beta_s/\nu} g_s(l/b^z, b^{1/\nu}t)$$
(26)

when lengths perpendicular to the surface are rescaled by a factor of b > 1. At the critical point t = 0 the decay exponent is given by $\eta_{\parallel} = 2\beta_s/vz$, which corresponds to the relation in (24), if

$$z = \beta_s + \overline{\beta}_s. \tag{27}$$

For the period-doubling sequence with $\beta_s = \overline{\beta}_s$, $\eta_{\parallel} = 1$, as observed. We note that the anisotropy exponent *z* has recently been analytically calculated for the corresponding Ising quantum chains [54] in accordance with (27). Thus we can conclude that for marginally aperiodic layered Ising models where the perturbation extends over the volume of the system, the systems become essentially anisotropic at the critical point and the anisotropy exponent can be expressed as the sum of the two surface magnetization exponents.

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Appendix

To prove equation (4) we start with the representation of H in (3) in the $\mu, \overline{\mu}$ basis:

$$H_{\mu,\overline{\mu}} = -\sum_{i=1}^{N-1} \lambda_i \mu_i \mu_{i+1} \delta_{\mu,\overline{\mu}} + \sum_{i=1}^N h_i \delta(\mu_i + \overline{\mu}_i) \prod_{j \neq i} \delta(\mu_j - \overline{\mu}_j).$$
(A1)

Then the matrix elements of the commutator $[T^2, H]$ are given by

$$(T^{2}H - HT^{2})_{\mu,\overline{\mu}} = -T^{2}_{\mu,\overline{\mu}} \left\{ \sum_{i=1}^{N} h_{i} \frac{\cosh(K_{2i-1}(\mu_{i} - \overline{\mu}_{i}) + K_{2i}(\mu_{i+1} + \overline{\mu}_{i+1}))}{\cosh(K_{2i-1}(\mu_{i} + \overline{\mu}_{i}) + K_{2i}(\mu_{i+1} + \overline{\mu}_{i+1}))} \right.$$

$$\times \frac{\cosh(K_{2i-3}(\mu_{i-1} + \overline{\mu}_{i-1}) + K_{2i-2}(\mu_{i} - \overline{\mu}_{i}))}{\cosh(K_{2i-3}(\mu_{i-1} + \overline{\mu}_{i-1}) + K_{2i-2}(\mu_{i} + \overline{\mu}_{i}))} + \sum_{i=1}^{N-1} \lambda_{i}\overline{\mu}_{i}\overline{\mu}_{i+1} - (\mu_{i} \leftrightarrow \overline{\mu}_{i}) \right\}.$$
(A2)

Here in the surface terms $K_0 = K_{-1} = K_{2N} = 0$. The term in the first sum on the right-hand side of (A2) can be rewritten using the identities $\sinh[a(\mu \pm \overline{\mu})] = (\mu \pm \overline{\mu})/2 \sinh 2a$ and $\tanh[a(\mu \pm \overline{\mu})] = (\mu \pm \overline{\mu})/2 \tanh 2a$ as

$$\begin{aligned} & [\mu_{i+1}\mu_i \tanh 2K_{2i} \sinh 2K_{2i-1} \cosh 2K_{2i-2} + \mu_i \mu_{i-1} \tanh 2K_{2i-3} \sinh 2K_{2i-2} \cosh 2K_{2i-1} \\ & +\overline{\mu}_{i+1}\mu_i \tanh 2K_{2i} \sinh 2K_{2i-1} \cosh 2K_{2i-2} \\ & +\mu_i \overline{\mu}_{i-1} \tanh 2K_{2i-3} \sinh 2K_{2i-2} \cosh 2K_{2i-1} - (\mu_i \leftrightarrow \overline{\mu}_i)]/2 \end{aligned}$$

so that we obtain for the commutator

$$[\mathbf{T}^{2}, \mathbf{H}]_{\mu,\overline{\mu}} = -\mathbf{T}_{\mu,\overline{\mu}}^{2} \left\{ \sum_{i=1}^{N-1} (\mu_{i+1}\mu_{i} - \overline{\mu}_{i+1}\overline{\mu}_{i}) \left[\frac{1}{2} S_{2i} S_{2i-1} \left(h_{i} \frac{C_{2i-2}}{C_{2i}} + h_{i+1} \frac{C_{2i+1}}{C_{2i-1}} \right) - \lambda_{i} \right] + \sum_{i=1}^{N-1} (\overline{\mu}_{i+1}\mu_{i} - \mu_{i+1}\overline{\mu}_{i}) \frac{1}{2} S_{2i} S_{2i-1} \left(h_{i} \frac{C_{2i-2}}{C_{2i}} - h_{i+1} \frac{C_{2i+1}}{C_{2i-1}} \right) \right\}.$$
(A3)

Then the commutator is zero if (4b) and (4c) are satisfied.

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