Surface Properties of Aperiodic Ising Quantum Chains

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(Phys. Rev. **B 57** (*Rap. Commun.*) 673-676 (1 January 1998))

We consider Ising quantum chains with a quenched aperiodic disorder of the coupling constants given through general substitution rules. The critical scaling behavior of several bulk and surface quantities is obtained by exact real space renormalization.

PACS numbers: 05.50.+q, 64.60.Ak, 75.10.Jm, 71.23.Ft

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Introduction. Ising quantum chains with aperiodically modulated coupling constants have been the topic of several recent publications,[1–6] see also papers cited in Ref. 7. These systems describe 2d classical Ising models, with couplings varying along layers, in the Hamiltonian limit and provide a non-trivial, but nevertheless easily accessible class of models to study the effect of aperiodic (dis)order on thermodynamic properties and critical behavior. Scaling arguments, put forward by Luck, lead to the following predictions on the relevance of aperiodic modulations:[8] The critical behavior is of Onsager-type as long as the fluctuations of the couplings are bounded, but resembles the randomly disordered case for unbounded fluctuations. Of particular interest is the marginal case with (in terms of the system size) logarithmically diverging fluctuations. Here, a non-universal scaling behavior is predicted with critical exponents that depend continuously on the coupling constants.

For sequences of coupling constants obtained from substitution rules, we demonstrated recently,[5] how Luck's criterion can be derived within an exact renormalization scheme, using a decimation procedure proposed in Ref. 4. This way, an exact expression for the scaling exponent z of the mass gap at criticality was obtained.

In this article, we show how the renormalization approach can be extended to describe the fermionic eigenvectors of the quantum chains. This leads to the exact determination of the critical scaling behavior of several bulk and surface quantities, like the bulk energy density or the surface magnetization. Quite recently, a similar derivation (using the decimation of Ref. 4) has been given for some special examples.[6] These results are contained as special cases here.

Ising quantum chains and substitution sequences. The Ising quantum chain is given by the Hamiltonian

$$\boldsymbol{H}_N = -\frac{1}{2}\left(\sum_{k=1}^{N} \varepsilon_k\, \boldsymbol{\sigma}_k^x \boldsymbol{\sigma}_{k+1}^x + \sum_{k=1}^{N} h_k \boldsymbol{\sigma}_k^z\right) \qquad (1)$$

with Pauli matrices $\boldsymbol{\sigma}_k^{x,z}$ acting on the kth site, and site-dependent transverse magnetic fields h_k. The site-dependent coupling constants ε_k shall be drawn from a set of values ε_{a_i}, where the label a_i is taken from an n-letter alphabet $\mathcal{A} = \{a_1, a_2, \ldots, a_n\}$. Initially, the field variables are chosen as $h_k \equiv 1$; but later on, as parameters in the renormalization transformation (RT), they become site-dependent and will correspondingly be labeled as $h_{k+1} = h_{a_i}$ (if $\varepsilon_k = \varepsilon_{a_i}$).

We choose the couplings according to sequences generated by iterated application of a substitution rule $\varrho : a_i \to w(a_i)$ on $\mathcal{A}$. Some important properties of the substitution chain are already contained in the corresponding $n \times n$ substitution matrix $\boldsymbol{M}_\varrho$, whose elements $(\boldsymbol{M}_\varrho)_{ij}$ give the number of letters a_j contained in the words $w(a_i)$. So, the asymptotic densities of the letters are given by the entries of the (statistically normalized) right eigenvector to the Perron-Frobenius (PF) eigenvalue $\lambda_1 = \lambda_{\mathrm{PF}}$ which is just the rescaling factor of the chain length. The fluctuations of the cumulated deviation of the couplings from the mean coupling grow as a power of the chain length, i.e. as N^ω, with a *wandering exponent* ω determined by the two largest eigenvalues (in modulus)

$$\omega = \frac{\log|\lambda_2|}{\log \lambda_{\mathrm{PF}}}\,. \qquad (2)$$

Thus fluctuations diverge for $|\lambda_2| \geq 1$, whereas the marginal case is connected to $|\lambda_2| = 1$.

The Ising quantum chain is critical, in the sense that the mass gap vanishes in the thermodynamic limit, if the geometric mean of the reduced couplings ε_j/h_j approaches 1 for $N \to \infty$. For couplings determined by substitution sequences, this is equivalent to the condition that the vector $\boldsymbol{y}$ of logarithms of the reduced couplings

$$\boldsymbol{y}_i = \log\left(\frac{h_{a_i}^2}{\varepsilon_{a_i}^2}\right) \qquad (i = 1, 2, \ldots, n) \qquad (3)$$

is perpendicular to the PF eigenvector of $\boldsymbol{M}_\varrho$.

For a general set of coupling constants ε_k, the quantum chain can be written as a free-fermion model via a Jordan-Wigner transformation and diagonalized canonically, resulting in[9]

$$\boldsymbol{H}_N = \sum_{q=1}^{N} \Lambda_q(\boldsymbol{\eta}_q^\dagger \boldsymbol{\eta}_q - \tfrac{1}{2}\mathbb{1}) + C_N \mathbb{1} \tag{4}$$

where $\boldsymbol{\eta}_q^\dagger$ and $\boldsymbol{\eta}_q$ are N fermionic creation and annihilation operators and where C_N is some constant. The dimensionless excitation energies Λ_q (which can be ordered as $0 \le \Lambda_1 \le \Lambda_2 \le \ldots \le \Lambda_N$) satisfy the linear difference equations

$$\Lambda_q \boldsymbol{\psi}_k^{(q)} = -\, h_k \boldsymbol{\phi}_k^{(q)} - \varepsilon_k \boldsymbol{\phi}_{k+1}^{(q)} \, , \tag{5a}$$

$$\Lambda_q \boldsymbol{\phi}_k^{(q)} = -\, \varepsilon_{k-1} \boldsymbol{\psi}_{k-1}^{(q)} - h_k \boldsymbol{\psi}_k^{(q)} \, . \tag{5b}$$

This corresponds to an eigenvalue problem of the matrix

$$\boldsymbol{\mathcal{H}} = \begin{pmatrix} 0 & h_1 & 0 & 0 & 0 & \cdots & 0 & \varepsilon_N \\ h_1 & 0 & \varepsilon_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \varepsilon_1 & 0 & h_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & h_2 & 0 & \varepsilon_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & h_{N-1} & 0 & \varepsilon_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & 0 & \varepsilon_{N-1} & 0 & h_N \\ \varepsilon_N & 0 & \cdots & 0 & 0 & 0 & h_N & 0 \end{pmatrix} \tag{6}$$

where $\varepsilon_N \equiv 0$ for *free* boundary conditions which are employed in the study of surface properties. Here, $\boldsymbol{\psi}_k^{(q)}$ and $\boldsymbol{\phi}_k^{(q)}$ are the even and the odd components of the eigenvector connected to the qth eigenvalue, respectively.

Renormalization scheme for fermionic eigenvectors. Following the presentation in Ref. 5, we now introduce the renormalization technique based on $\boldsymbol{\mathcal{S}}$-transfer matrices and their star-products.[10] For technical reasons, we restrict the discussion to substitution rules of the form

$$\varrho : a_i \to a_i w_i \tag{7}$$

where w_i are n arbitrary words in the n-letter alphabet $\mathcal{A}$, and only comment on the extension to the general case. We introduce $\boldsymbol{\mathcal{S}}$-matrices that transform the components of the eigenvectors of Eq. (6) as

$$\begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\phi}_{l+1} \end{pmatrix} = \boldsymbol{\mathcal{S}}_{k|l} \begin{pmatrix} \boldsymbol{\phi}_{k+1} \\ \boldsymbol{\psi}_l \end{pmatrix} \tag{8}$$

with

$$\boldsymbol{\mathcal{S}}_{k|l} = \boldsymbol{\mathcal{S}}_{k|k+1} * \boldsymbol{\mathcal{S}}_{k+1|k+2} * \ldots * \boldsymbol{\mathcal{S}}_{l-1|l} \, , \tag{9}$$

where the $*$-product of two 2×2 matrices is defined as

$$\begin{pmatrix} e & \bar{e} \\ r & \rho \end{pmatrix} * \begin{pmatrix} \rho_1 & r_1 \\ \bar{o} & o \end{pmatrix} = \begin{pmatrix} e & 0 \\ 0 & o \end{pmatrix} + \frac{1}{1-\rho\rho_1} \begin{pmatrix} \bar{e}r\rho_1 & \bar{e}r_1 \\ \bar{o}r & \bar{o}r_1\rho \end{pmatrix} . \tag{10}$$

According to Eq. (6), the elementary $\boldsymbol{\mathcal{S}}$-matrices are

$$\boldsymbol{\mathcal{S}}_{k|k+1} = \begin{pmatrix} \varepsilon_k^{-1}\Lambda & -\varepsilon_k^{-1} h_{k+1} \\ -\varepsilon_{k+1}^{-1} h_{k+1} & \varepsilon_{k+1}^{-1}\Lambda \end{pmatrix} \tag{11}$$

where Λ denotes an eigenvalue of $\boldsymbol{\mathcal{H}}$. In order to establish the RT, the fields and vector components are labeled according to the locally varying coupling constants. Furthermore, two additional asymmetry coefficients $\kappa_{a_i}^{\pm}$ have to be introduced for every letter $a_i \in \mathcal{A}$. This way, we obtain n^2 different elementary $\boldsymbol{\mathcal{S}}$-transfer matrices through

$$\begin{pmatrix} \boldsymbol{\psi}_{a_i,k} \\ \boldsymbol{\phi}_{a_j,k+2} \end{pmatrix} = \boldsymbol{\mathcal{S}}_{a_i|a_j} \begin{pmatrix} \boldsymbol{\phi}_{a_i,k+1} \\ \boldsymbol{\psi}_{a_j,k+1} \end{pmatrix} \tag{12}$$

where the second label refers to the position, and where

$$\boldsymbol{\mathcal{S}}_{a_i|a_j} = \begin{pmatrix} \varepsilon_{a_i}^{-1}\kappa_{a_i}^{+}\Lambda & -\varepsilon_{a_i}^{-1} h_{a_i} \\ -\varepsilon_{a_j}^{-1} h_{a_i} & \varepsilon_{a_j}^{-1}\kappa_{a_i}^{-}\Lambda \end{pmatrix} . \tag{13}$$

Unlike the fields or the couplings, the eigenvector components depend not only through the a_i, but also *explicitly* on the position, so we have to keep the labels here. The RT now reverses the substitution steps by building $*$-products of $\boldsymbol{\mathcal{S}}$-transfer matrices corresponding to the words w_i given by the substitution rule. The resulting RT's of $\kappa_{a_i}^{\pm}\Lambda$ and h_{a_i} have been described in Ref. 5. For coupling constants fulfilling the criticality condition, the vector $\boldsymbol{y}$ of logarithms of the reduced couplings is found to scale with the next-to-leading eigenvalue λ_2 of $\boldsymbol{M}_\varrho$. Especially, in the marginal case with $\lambda_2 = 1$, $\boldsymbol{y}$ converges to an eigenvector corresponding to an eigenvalue 1 of the *transpose* $\boldsymbol{M}_\varrho^t$ of the substitution matrix.

Let us now concentrate on the RT equations for the vector components of $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$. Since iterated $*$-multiplications of the $\boldsymbol{\mathcal{S}}$-matrices act as a pure decimation on the vector components, the remaining components of the renormalized vectors $\tilde{\boldsymbol{\psi}}$ and $\tilde{\boldsymbol{\phi}}$ differ from the original ones only through relabeling and a normalization factor

$$\tilde{\boldsymbol{\psi}}_m = C_\psi \, \boldsymbol{\psi}_k \, , \quad \tilde{\boldsymbol{\phi}}_{m+1} = C_\phi \, \boldsymbol{\phi}_{k+1} \, , \tag{14}$$

with $k/m \to \lambda_{\mathrm{PF}}$ and normalization constants $C_{\psi,\phi}$ such that both $\tilde{\boldsymbol{\psi}}$ and $\tilde{\boldsymbol{\phi}}$ are normalized to one. We now proceed to determine the scaling behavior of these normalization constants at the critical point $\Lambda \equiv 0$. As the diagonal elements of the $\boldsymbol{\mathcal{S}}$-matrices vanish to leading order in Λ, the RT equations for $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ decouple at the critical point and can be considered separately. By taking successive $*$-products along the words w_i, the *original* eigenvector components may now be expressed in terms of the *renormalized* ones

$$\begin{pmatrix} \boldsymbol{\psi}_{a_i,k} \\ \boldsymbol{\phi}_{w_i^j,k+j+1} \end{pmatrix} = \boldsymbol{\mathcal{S}}_{a_i|w_i^j} \begin{pmatrix} \boldsymbol{\phi}_{a_i,k+1} \\ \boldsymbol{\psi}_{w_i^j,k+j} \end{pmatrix} \tag{15}$$

where w_i^j denotes the jth letter of w_i and

$$\boldsymbol{\mathcal{S}}_{a_i|w_i^j} = \boldsymbol{\mathcal{S}}_{a_i|w_i^1} * \boldsymbol{\mathcal{S}}_{w_i^1|w_i^2} * \cdots * \boldsymbol{\mathcal{S}}_{w_i^{j-1}|w_i^j} \, . \tag{16}$$

Explicitly, we obtain the following relations

$$\boldsymbol{\phi}_{a_i,k+1}^2 = (C_\phi^{-1}\tilde{\boldsymbol{\phi}}_{a_i,m+1})^2 \, , \tag{17a}$$

$$\boldsymbol{\phi}_{w_i^j,k+j+1}^2 = \frac{h_{a_i}^2 h_{w_i^1}^2 \ldots h_{w_i^{j-1}}^2}{\varepsilon_{w_i^1}^2 \varepsilon_{w_i^2}^2 \ldots \varepsilon_{w_i^j}^2} (C_\phi^{-1}\tilde{\boldsymbol{\phi}}_{a_i,m+1})^2 \, , \tag{17b}$$

and

$$\boldsymbol{\psi}^2_{a_i,k} = (C_\psi^{-1}\tilde{\boldsymbol{\psi}}_{a_i,m})^2 \ , \tag{18a}$$

$$\boldsymbol{\psi}^2_{w_i^j,k+j} = \frac{\varepsilon^2_{a_i}\varepsilon^2_{w_i^1}\cdots\varepsilon^2_{w_i^{j-1}}}{h^2_{a_i}h^2_{w_i^1}\cdots h^2_{w_i^{j-1}}}(C_\psi^{-1}\tilde{\boldsymbol{\psi}}_{a_i,m})^2 \ , \tag{18b}$$

with the reduced couplings at their fixed point values. In order to derive the renormalization factor of C_ψ and C_ϕ, we now perform partial sums of the squared vector entries, according to their additional labels a_i,

$$\boldsymbol{\Psi}_i = \sum_k \boldsymbol{\psi}^2_{a_i,k} \ , \quad \boldsymbol{\Phi}_i = \sum_k \boldsymbol{\phi}^2_{a_i,k} \ . \tag{19}$$

For these vectors $\boldsymbol{\Psi}$ and $\boldsymbol{\Phi}$, the RT at the critical point yields a simple matrix form

$$C_\psi^2 \boldsymbol{\Psi} = \boldsymbol{M}^\psi \tilde{\boldsymbol{\Psi}} \ , \quad C_\phi^2 \boldsymbol{\Phi} = \boldsymbol{M}^\phi \tilde{\boldsymbol{\Phi}} \ , \tag{20}$$

where

$$\boldsymbol{M}^\psi_{ij} = \sum_{k=1}^{|w_i|} \delta_{w_i^k,a_j} \frac{h^2_{w_i^k}}{h^2_{a_i}} \frac{\varepsilon^2_{a_i}}{\varepsilon^2_{w_i^k}} \prod_{l=1}^{k} \frac{\varepsilon^2_{w_i^l}}{h^2_{w_i^l}} + \delta_{a_i,a_j} \ , \tag{21a}$$

$$\boldsymbol{M}^\phi_{ij} = \sum_{k=1}^{|w_i|} \delta_{w_i^k,a_j} \frac{h^2_{a_i}}{h^2_{w_i^k}} \prod_{l=1}^{k} \frac{h^2_{w_i^l}}{\varepsilon^2_{w_i^l}} + \delta_{a_i,a_j} \ . \tag{21b}$$

Since all components of the vectors $\boldsymbol{\Psi}$, $\boldsymbol{\Phi}$ and the matrices $\boldsymbol{M}^{\psi,\phi}$ are positive, the vectors converge to the PF eigenvectors of $\boldsymbol{M}^{\psi,\phi}$ under iteration of the RT. We formally conclude, for the normalization constants,

$$C_\psi = \sqrt{\mu^\psi} \ , \quad C_\phi = \sqrt{\mu^\phi} \ , \tag{22}$$

where $\mu^{\psi,\phi}$ are the PF eigenvalues of $\boldsymbol{M}^{\psi,\phi}$. At this point, we can make contact to the RT of the lowest fermionic excitations considered in Ref. 5. To this end, we transform $\boldsymbol{M}^{\psi,\phi}$ under conservation of the spectrum according to $\boldsymbol{M}^- = (\boldsymbol{T}^\psi)^{-1}\boldsymbol{M}^\psi\boldsymbol{T}^\psi$ and $\boldsymbol{M}^+ = (\boldsymbol{T}^\phi)^{-1}\boldsymbol{M}^\phi\boldsymbol{T}^\phi$ with diagonal transformation matrices $\boldsymbol{T}^\psi_{ij} = (\varepsilon_{a_i}/h_{a_i})^2\delta_{i,j}$ and $\boldsymbol{T}^\phi_{ij} = h^2_{a_i}\delta_{i,j}$. We find

$$\boldsymbol{M}^\pm_{ij} = \sum_{k=1}^{|w_i|} \delta_{w_i^k,a_j} \prod_{l=1}^{k} \left(\frac{h^2_{w_i^l}}{\varepsilon^2_{w_i^l}}\right)^{\pm 1} + \delta_{a_i,a_j} \ . \tag{23}$$

If $\mu^- \equiv \mu^\psi$ and $\mu^+ \equiv \mu^\phi$ denote the leading eigenvalues of $\boldsymbol{M}^\pm$, note that $\mu^-(\{\varepsilon_{a_i}/h_{a_i}\}) = \mu^+(\{h_{a_i}/\varepsilon_{a_i}\})$.

For substitution chains with bounded or marginal fluctuations of the coupling constants, however, these are exactly the forms of the RT-matrices for the fermion frequencies [see Eqs. (3.21) and (3.25) in Ref. 5]. For comparison, recall that one has

$$\prod_{l=1}^{|w_i|} \frac{h^2_{w_i^l}}{\varepsilon^2_{w_i^l}} = 1 \tag{24}$$

for $|\lambda_2| \leq 1$. The lowest fermion frequencies transform as $\tilde{\Lambda} = \sqrt{\mu^+\mu^-}\Lambda$, resulting in the scaling behavior[5]

$$\Lambda_q = x_q N^{-z} \ , \quad z = \frac{\log(\mu^+\mu^-)}{2\log\lambda_{\rm PF}} \ . \tag{25}$$

The extension of the RT to general substitution rules has been described in Ref. 5; it can be performed along the same lines here. Generally, the substitution rule has to be redefined as a function acting on *pairs* of letters, generating the same chain. General $\boldsymbol{\mathcal{S}}$-matrices $\boldsymbol{\mathcal{S}}_{a_i|a_j}$ contain fields and asymmetry parameters, and act on vector components, all carrying a double label $(\ldots)_{a_ia_j}$. The RT of the eigenvector components can again be given as a matrix equation (of dimension n^2) and identified with the RT of the fermionic excitations as above.

Results on critical scaling. The *surface magnetization* m_{s1} (on the *left* surface) can be obtained from the large distance limit of the spin-correlation function at the surface, leading to the expression[11,12]

$$m_{s1} = \langle 1|\sigma_1^x|0\rangle = \boldsymbol{\phi}_1^{(1)} \ . \tag{26}$$

Here, $|1\rangle = \boldsymbol{\eta}_1^\dagger|0\rangle$ is the lowest excited state which becomes degenerate with the ground state in the ordered phase,[11] and the last equality is obtained upon expressing σ_1^x in terms of the fermions. Thus, m_{s1} is simply the first entry of the normalized eigenvector $\boldsymbol{\phi}^{(1)}$ of the lowest fermionic excitation. Since $\tilde{\boldsymbol{\phi}}_1^{(1)} = \sqrt{\mu^+}\boldsymbol{\phi}_1^{(1)}$ [see Eqs. (14) and (22), and remember that $\mu^+ \equiv \mu^\phi$], we obtain the surface magnetization exponent β_{s1} through

$$m_{s1} \sim N^{-\beta_{s1}/\nu} \ , \quad \beta_{s1} = \frac{\log\mu^+}{2\log\lambda_{\rm PF}} \ . \tag{27}$$

Note that β_{s1} is given by the scaling exponent here, since the correlation length exponent (along the layers of the 2d classical model) retains its unperturbed value $\nu = 1$.[1,3] Using a method of Ref. 12, the surface magnetization of several substitution sequences was calculated before.[1] However, it seems impossible to extend this method to the general case. Recently, the results of Ref. 1 have also been rederived[6] using real space renormalization.

For substitution chains with bounded fluctuations (and second largest eigenvalue of the substitution matrix $|\lambda_2| < 1$), like e.g. the Fibonacci chain, all reduced couplings converge to the critical value of the uniform chain $\varepsilon_{a_i}/h_{a_i} \to 1$ and we find $\boldsymbol{M}^+ = \boldsymbol{M}^- = \boldsymbol{M}_\varrho$, thus $\mu^+ = \lambda_{PF}$ and β_{s1} takes its Onsager value $\beta_{s1} = 1/2$.

For two-letter substitution chains, which always can be generated by a substitution rule of the form (7),[5] an explicit result can be obtained also for the marginal case ($\lambda_2 = 1$). Here, the PF eigenvalue of $\boldsymbol{M}^\pm$ coincides with the trace of these matrices,[5] resulting in

$$\beta_{s1} = \frac{\log(\boldsymbol{M}^+_{11} + \boldsymbol{M}^+_{22} - 1)}{2\log\lambda_{\rm PF}} \tag{28}$$

where $\boldsymbol{M}^+_{11}$ and $\boldsymbol{M}^+_{22}$ are given in Eq. (23). In general, β_{s1} depends on the coupling constants through $r < n$

independent parameters, where r is the dimension of the (joined) eigenspace to eigenvalues $|\lambda| = 1$ of $\boldsymbol{M}_\varrho$.

For substitution chains with fluctuations that diverge with a power-law, the situation is slightly more complex. Here, the reduced couplings scale as $\exp(\boldsymbol{y}_i N^\omega)$; and since $\boldsymbol{y}$ always contains components of different sign, part of them flow to infinity under the RT, while others converge to zero. For the RT of $C_{\phi,\psi}$, consider the behavior of the entries of $\boldsymbol{M}^\pm$ for *iterated* substitution steps ϱ^n. According to Eq. (23), all entries are polynomials of the reduced couplings. Now, two cases have to be distinguished — depending not only on the substitution matrix, but on the detailed form of the substitution itself. Generically, all entries are finally dominated by reduced couplings that flow to infinity under the RT. This is always the case if the cumulated deviation of any type of coupling from its mean is unbounded in positive *and* negative direction. In this case, m_{s1} will finally scale as $\exp(-cN^\omega)$, with c depending on the coupling constants.

There are, however, special cases, where the cumulated deviation does not diverge symmetrically, but, depending on the initial word (seed) of the inflation, only in positive (or in negative) direction. As a simple example, consider the two-letter substitution rule

$$\varrho : \begin{array}{lcl} a & \rightarrow & aaab \\ b & \rightarrow & bbba \end{array} . \tag{29}$$

Let $\sharp_{a,b}(n)$ be the number of a, b's among the first n letters of the limit chain; we find $1/2$ as the asymptotic frequency for both letters. Choosing, however, the single letter a as the seed, the number $\sharp_a(n) - \sharp_b(n)$ is unbounded, but *positive* for any n, thus the fluctuations are bounded from below for this chain. For the corresponding matrices $\boldsymbol{M}^\pm$, this means that, for given couplings, certain entries do not diverge, but finally tend to a finite value or to zero. Starting with the appropriate seed, this results in a *finite* surface magnetization m_{s1} (on one side of the chain), also at criticality. This explains the (unusual) behavior that has been observed in Ref. 2 for a special substitution rule.

The *surface magnetization* m_{s2} on the *right* surface follows, after an *inversion* of the substitution rule to $\bar{\varrho} : a_i \rightarrow \bar{w}_i a_i$, through the same procedure as described above. The RT for the vector components reads

$$\begin{pmatrix} \boldsymbol{\psi}_{w_i^j,k-j} \\ \boldsymbol{\phi}_{a_i,k+1} \end{pmatrix} = \boldsymbol{\mathcal{S}}_{w_i^j|a_i} \begin{pmatrix} \boldsymbol{\phi}_{w_i^j,k-j+1} \\ \boldsymbol{\psi}_{a_i,k} \end{pmatrix} , \tag{30}$$

and we deduce the same relations as above *with all reduced couplings inverted*, i.e., $\varepsilon_{a_i}/h_{a_i} \rightarrow h_{a_i}/\varepsilon_{a_i}$. Thus

$$\beta_{s2}\big(\{\frac{\varepsilon_{a_i}}{h_{a_i}}\}\big) = \beta_{s1}\big(\{\frac{h_{a_i}}{\varepsilon_{a_i}}\}\big) = \frac{\log \mu^-}{2 \log \lambda_{\rm PF}} . \tag{31}$$

This generalizes a symmetry in scaling of m_{s1} and m_{s2}[3,6] also to substitution chains where this symmetry is not obvious from the chain geometry, and to general n-letter substitutions. We also conclude, for arbitrary n-letter substitution chains with marginal (or bounded) fluctuations of the coupling constants, that

$$z = \beta_{s1} + \beta_{s2} \tag{32}$$

as conjectured in Ref. 3 and argued-for in Ref. 6.

The *surface energy density* can be obtained from the two lowest fermionic excitations as follows[3]

$$e_{s1} \sim (\Lambda_2 - \Lambda_1)\, \boldsymbol{\phi}_1^{(1)} \boldsymbol{\phi}_1^{(2)} . \tag{33}$$

Hence, we find the scaling behavior $e_{s1,2} \sim N^{-z-2\beta_{s1,2}}$ conjectured in Ref. 3 on the basis of numerical results.

The *bulk energy density* on site j follows from the matrix element[3]

$$e_k = \left| \boldsymbol{\psi}_k^{(1)} \boldsymbol{\phi}_k^{(2)} - \boldsymbol{\psi}_k^{(2)} \boldsymbol{\phi}_k^{(1)} \right| . \tag{34}$$

Thus, $\tilde{e}_m = \sqrt{\mu^+\mu^-} e_k$ and $e_{N/k} \sim N^{-z}$, as had also been conjectured in Ref. 3.

Conclusions. We have demonstrated how the bulk and surface critical behavior of aperiodic Ising quantum chains (or, equivalently, of aperiodically layered, two-dimensional classical Ising systems) obtained from general substitution rules can be derived by exact real space renormalization. The results corroborate a number of conjectures on scaling laws for these systems and generalize previous results obtained for special examples. An exact calculation of the bulk magnetization seems to be more difficult and remains an open problem.

Acknowledgement. The authors thank M. Baake for discussions and helpful comments.

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