Aperiodic Ising Quantum Chains

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Abstract

Some years ago, Luck proposed a relevance criterion for the effect of aperiodic disorder on the critical behaviour of ferromagnetic Ising systems. In this article, we show how Luck's criterion can be derived within an exact renormalization scheme for Ising quantum chains with coupling constants modulated according to substitution rules. Luck's conjectures for this case are confirmed and refined. Among other outcomes, we give an exact formula for the correlation length critical exponent for arbitrary two-letter substitution sequences with marginal fluctuations of the coupling constants.

1 Introduction

The influence of aperiodic (dis-)order on the thermodynamic properties and the critical behaviour of spin systems has been an active research area, particularly since the discovery of quasicrystals in 1984. In view of the many articles existing, we cannot give proper credit to all contributors; instead, we would like to refer the reader to a recent review [13] which contains a rather complete bibliography on this subject. For ferromagnetic Ising systems, heuristic scaling arguments, put forward by Luck [18], lead to qualitative predictions on the relevance of disorder implemented through an aperiodic variation of the coupling constants which go beyond the original relevance-irrelevance criterion of Harris [14]. For the Ising quantum chain (IQC), or the equivalent $2d$ classical Ising model [17] with layered disorder, this relevance criterion reads as follows: The critical behaviour is of Onsager-type as long as the fluctuations in the sequence of coupling constants are bounded, whereas for unbounded fluctuations the critical singularities resemble those of the randomly disordered case. This behaviour had first been conjectured by Tracy [24] on ths basis of his results for two different examples of three-letter substitution rules. Of

particular interest is the marginal case with logarithmically (in the system size) diverging fluctuations. Here, the critical exponents are predicted to depend continuously on the coupling constants [18].

Meanwhile, some exact results were obtained for substitution chains with marginal fluctuations of the couplings. For a number of substitution chains, the surface magnetisation critical exponent could be calculated [26, 6, 7, 5]; and, recently, the correlation length critical exponent was derived for two special substitution rules using an exact renormalization approach [15]. All these results are in accordance with Luck's predictions.

The real space renormalization method we use in this article is based on the decimation process introduced in Ref. [15]. Our setup is quite different, though; and in particular we are going to show how *arbitrary* substitution rules can be analysed in terms of S-matrices and their star-product formalism. In this way, the dependence of the critical behaviour on the nature of the fluctuations can be derived explicitly. The analysis is carried out in detail for two-letter substitution chains, with the result that Luck's relevance criterion emerges from the renormalization relations in a natural way. An extended renormalization scheme for the most general case of n-letter substitution rules is presented in an Appendix and discussed for certain examples. For infinite classes of substitution chains with marginal fluctuations, including the two-letter chains, an analytic expression for the correlation length critical exponent is given.

This article is organised as follows. In Sec. 2, we give a brief outline of the model, including some introductory remarks on substitution rules and on properties of the corresponding substitution sequences. Then, in Sec. 3, we introduce the renormalization transformation for a restricted class of n-letter substitution chains, comprising all two-letter substitution chains. The dependence of the renormalization flow on the fluctuations of the couplings is shown and the consequences are discussed in detail. Subsequently, in Sec. 4, we summarise the implications of our results for the critical properties of the IQC for the three different types of fluctuations in the sequence of the coupling constants. Our conclusions and an outlook on future developments are presented in Sec. 5. The paper contains two Appendices related to the content of Sec. 3: In Appendix A, the solution of the eigenvalue problem for the case of a two-letter substitution sequence is derived; and finally, generalising the discussion of Sec. 3, the renormalization transformation for arbitrary n-letter substitution rules is explained in Appendix B.

2 Ising quantum chain and substitution sequences

The IQC in a transverse magnetic field is defined by the Hamiltonian

$$H_N = -\frac{1}{2}\left(\sum_{j=1}^{N} \varepsilon_j\, \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^{N} h_j \sigma_j^z\right) \tag{2.1}$$

acting on the tensor-product space $\bigotimes_{j=1}^{N} \mathbb{C}^2 \cong \mathbb{C}^{2^N}$. Here, the h_j denote the transverse fields at the sites. The ε_j are site-dependent coupling constants, and the operators $\sigma_j^{x,z}$ denote Pauli's matrices acting on the jth site. In what follows, we consider closed chains with *periodic* boundary conditions which are defined by $\sigma_{N+1}^x = \sigma_1^x$; various other kinds of boundary conditions can be chosen without changing the key results.

For a general set of coupling constants ε_j and fields h_j, the IQC can be written as a free-fermion model via a Jordan-Wigner transformation and can then be diagonalised by a Bogoljubov-Valatin transformation, resulting in [16]

$$H_N = \sum_{q=1}^{N} \Lambda_q (\eta_q^\dagger \eta_q - \tfrac{1}{2}) + C \tag{2.2}$$

where $\eta_q^\dagger$, η_q are N fermionic creation and annihilation operators and C is some constant. The dimensionless excitation energies Λ_q (which can be chosen to be positive and ordered, i.e., $\Lambda_N \geq \ldots \geq \Lambda_2 \geq \Lambda_1 \geq 0$, while properly adjusting the constant C) satisfy the linear difference equations

$$\begin{aligned} \Lambda_q \Psi_q(j) &= -h_j \Phi_q(j) - \varepsilon_j \Phi_q(j+1) \,, \\ \Lambda_q \Phi_q(j) &= -\varepsilon_{j-1} \Psi_q(j-1) - h_j \Psi_q(j) \,. \end{aligned} \tag{2.3}$$

Normally, one proceeds by eliminating either Ψ or Φ. In this way, the problem of diagonalising the $2^N \times 2^N$ matrix H_N can be reduced to the diagonalisation of an $N \times N$ matrix. From the set of N eigenvalues (fermion frequencies) Λ_q of the latter, the total spectrum of the complete Hamiltonian H_N is recovered by considering the sums of the elements of any of its 2^N subsets. For periodic boundary conditions, the situation is in fact a little more complicated; in order to avoid the appearance of a non-local number operator in the fermionic Hamiltonian one has to consider so-called *mixed sector* Hamiltonians. These are obtained by combining the *even* sector (with respect to the operator $\prod_{j=1}^{N} \sigma_j^z$ that commutes with H_N) of the Hamiltonian (2.1) with *periodic* boundary conditions with the *odd* sector of the same Hamiltonian with *antiperiodic* boundary conditions (defined by $\sigma_{N+1}^x = -\sigma_1^x$), and vice versa [2, 11].

The IQC is equivalent to the $2d$ classical Ising model with a layered modulation of the interactions [17]. The correspondence shows up through an extremely anisotropic limit (also called the τ-continuum limit [10]) of the coupling constants of the latter, which is believed not to alter the critical behaviour. Explicitly, one establishes the following relations: The *temperature* T of the classical model corresponds to the *transverse field* h of the quantum chain, the *free energy* translates into the *ground-state energy* and the counterpart of the *correlation length* $\xi_\parallel$ *parallel* to the layers is the *inverse mass gap* $(E_1 - E_0)^{-1}$ of the IQC. In our setting, the mass gap is just given by the modulus of the smallest fermionic excitation Λ_1 of (2.2). According to finite-size scaling, we thus expect

a scaling behaviour of Λ_1 at the critical point as

$$\Lambda_1(N) = m^{\nu_\parallel/\nu_\perp}\Lambda_1(mN) =: m^z \Lambda_1(mN)\,, \tag{2.4}$$

provided the correlation length scales with a power law at all. Hereby, the scaling exponent z translates into the correlation length critical exponent $\nu_\parallel$ parallel to the layers in terminology of the $2d$ statistical system, while $\nu_\perp$ retains its unperturbed Onsager value $\nu_\perp = 1$.

The Hamiltonian (2.1) is *critical* (in the sense that the energy gap in the excitation spectrum vanishes, i.e., $\Lambda_1 = 0$) in the thermodynamic limit if the *geometric mean* (rather than the arithmetic mean) of the couplings, normalized by the variables of the transverse field, is equal to one, i.e.,

$$\lim_{N\to\infty} \left| \frac{\varepsilon_1}{h_1} \cdots \frac{\varepsilon_N}{h_N} \right|^{1/N} \;=\; 1\,, \tag{2.5}$$

compare Ref. [20]. The repetitive structure of the substitution sequences we are going to consider guarantees that the mean is well-defined [21, 19]. Let us now assume that the coupling constants ε_j $(j = 1, 2, \ldots, N)$ are chosen from a set of n possible values ε_m $(m = 1, 2, \ldots, n)$, the value ε_m occuring with a frequency p_m (where $\sum_{m=1}^{n} p_m = 1$). For simplicity, we take the field to be constant, i.e., $h_j \equiv h = 1$. Then, condition (2.5) can be fulfilled by choosing n positive real numbers $r_1, r_2, \ldots, r_n$ with $r_1 \cdot r_2 \cdot \ldots \cdot r_n = 1$, and setting the couplings to

$$\varepsilon_m \;=\; r_m^{p/p_m}\,, \tag{2.6}$$

where $p = p_1 \cdot p_2 \cdot \ldots \cdot p_n$. Unless stated otherwise, this parametrisation of the critical surface will be used in the sequel.

Substitution sequences

Let us now consider coupling constants ε_j drawn from a set of values ε_α, where the label $\alpha \in \mathcal{A}$ runs over the letters of a (finite) n-letter alphabet $\mathcal{A}$. We choose the couplings ε_j according to sequences generated by iterated application of a substitution rule $\varrho : \alpha \to w_\alpha$ on $\mathcal{A}$. For the introduction of the concept and some notation, consider a simple example on a two-letter alphabet $\mathcal{A} = \{a, b\}$:

$$\varrho^{(k)} : \begin{array}{ccc} a & \to & ab \\ b & \to & a^k \end{array}\,, \qquad \boldsymbol{M}_{\varrho^{(k)}} = \begin{pmatrix} 1 & k \\ 1 & 0 \end{pmatrix}\,, \qquad \lambda_\pm^{(k)} = \frac{1 \pm \sqrt{4k+1}}{2}\,. \tag{2.7}$$

We start with an initial word, e.g. $\mathcal{W}_0 = a$, and define $\mathcal{W}_{m+1} = \varrho^{(k)}(\mathcal{W}_m)$. $\boldsymbol{M}_{\varrho^{(k)}}$ denotes the corresponding substitution matrix (whose elements count the number of letters a and b in the words w_a and w_b), which has the eigenvalues $\lambda_\pm^{(k)}$. The entries of the, statistically normalized, (right) eigenvector $\boldsymbol{v}_{\mathrm{PF}}$, corresponding to the Perron-Frobenius eigenvalue $\lambda_{\mathrm{PF}} = \lambda_+^{(k)}$, give the frequencies of the letters in the limit word $\mathcal{W}_\infty$. In order to ensure

that, starting from any seed, the letter frequencies converge to unique, positive values in the limit chain, we restrict ourselves to *primitive* substitution rules ϱ throughout this paper. For the corresponding substitution matrices $\boldsymbol{M}_\varrho$, this means that the entries of $\boldsymbol{M}_\varrho^\ell$ are *strictly positive* for any integer $\ell > \ell_0$ (and a suitably chosen finite $\ell_0 \geq 0$). This is obviously true for the examples (2.7).

Associated to a word $\mathcal{W}_m$ of length (i.e., number of letters) $N = |\mathcal{W}_m|$, one obtains finite (closed) quantum chains with N sites by setting $\varepsilon_j = \varepsilon_a$ whenever the jth letter of the word $\mathcal{W}_m$ is an a, and $\varepsilon_j = \varepsilon_b$ otherwise, the final letter of $\mathcal{W}_m$ determining the coupling between the last and the first spin in the chain. While λ_{PF}, the largest eigenvalue of the substitution matrix, describes the asymptotic scaling of the chain length with the number of iterations m, $N \sim (\lambda_{\mathrm{PF}})^m$, the *fluctuation* behaviour of the exchange couplings is connected to the second-largest eigenvalue λ_2 (where it is the *modulus* of the eigenvalue that matters, hence by "second-largest eigenvalue" we always refer to the eigenvalue with the second-largest absolute value). In order to quantify the fluctuations, let us define

$$g_{\mathcal{W}} = \sum_{\alpha \in \mathcal{W}} (\varepsilon_\alpha - \bar{\varepsilon}) \tag{2.8}$$

where $\bar{\varepsilon}$ is the average coupling in the limit chain. Fluctuations stay *bounded* as long as $|\lambda_2| < 1$, but for $|\lambda_2| > 1$ they grow with iterated substitutions as a power of the chain length, $g_{\mathcal{W}} \sim N^\beta$, governed by the so-called *wandering exponent* β that is given by

$$\beta = \frac{\log |\lambda_2|}{\log \lambda_{\mathrm{PF}}} \,. \tag{2.9}$$

In the limiting case $|\lambda_2| = 1$, $|g_{\mathcal{W}}|$ stays constant when we prolong the chain by complete iteration steps. Generically, however, finite fluctuations within the substitutes w_α of the letters α will increase the total fluctuation in the vicinity of these points by a certain amount δ: $g_{\widetilde{\mathcal{W}}} \geq g_{\mathcal{W}} + \delta$ for some word $\widetilde{\mathcal{W}}$ with $\left| |\widetilde{\mathcal{W}}| - |\varrho(\mathcal{W})| \right| \leq \Delta$ and fixed Δ. By repeated use of this argument, we thus expect fluctuations that *diverge logarithmically* with the length of the chain (since the length grows exponentially with the number of iterations), see also Ref. [9]. On the other hand, the same argument also shows that, in this case, the fluctuation behaviour is not completely determined by the *substitution matrix*, but may also depend on the details of the actual *substitution rule* [12]; and for special choices the fluctuations may still stay bounded even though the second-largest eigenvalue is $|\lambda_2| = 1$.

Coming back to our examples (2.7), let us concentrate on the three cases $k = 1$ (which yields the famous *Fibonacci sequence*), $k = 2$ (the *period-doubling sequence*), and $k = 3$ (the *binary non-Pisot sequence*). As the second-largest eigenvalues of the substitution matrices $\boldsymbol{M}_{\varrho^{(k)}}$ fulfill $|\lambda_-^{(1)}| < 1$, $|\lambda_-^{(2)}| = 1$, and $|\lambda_-^{(3)}| > 1$, this includes an example of bounded fluctuations ($k = 1$), a marginal case with logarithmically divergent fluctuations ($k = 2$) and an example of strong fluctuations ($k = 3$), hence all three interesting cases

are illustrated [12]. Another substitution chain that is referred to several times in the text is the celebrated *Thue-Morse sequence*

$$\varrho^{(\mathrm{TM})}: \begin{array}{ccc} a & \to & ab \\ b & \to & ba \end{array}, \qquad \boldsymbol{M}_{\varrho^{(\mathrm{TM})}} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \lambda_+^{(\mathrm{TM})} = 2\,, \quad \lambda_-^{(\mathrm{TM})} = 0\,. \tag{2.10}$$

3 Renormalization transformation

Rather than reducing the set of linear equations (2.3) to N dimensions, we proceed (as does Ref. [15]) with a direct treatment as a $2N$-dimensional eigenvalue problem of the real symmetric matrix

$$\mathcal{H} = \begin{pmatrix} 0 & h_1 & 0 & 0 & 0 & \cdots & 0 & \varepsilon_N \\ h_1 & 0 & \varepsilon_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \varepsilon_1 & 0 & h_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & h_2 & 0 & \varepsilon_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & h_{N-1} & 0 & \varepsilon_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & 0 & \varepsilon_{N-1} & 0 & h_N \\ \varepsilon_N & 0 & \cdots & 0 & 0 & 0 & h_N & 0 \end{pmatrix}. \tag{3.1}$$

Since $\mathcal{H}$ is symmetric and bipartite[1], the eigenvalues occur in real pairs of opposite sign. But changing the sign of an eigenvalue simply means interchanging the corresponding creation and annihilation operators in Eq. (2.2), thus we can restrict ourselves to the positive part of the spectrum. In what follows, we concentrate on the case of a constant field $h_j \equiv h$, where we may set $|h| = 1$ by an appropriate choice of the energy scale. Of course, one cannot possibly expect analytical results for an arbitrary sequence of couplings. However, for *substitution* sequences, more can be said using an exact renormalization scheme, and, for an interesting class of chains with marginal fluctuations, the scaling exponent z (2.4) can be determined exactly and given in a closed form.

Consider now sequences of couplings chosen according to a substitution rule

$$\varrho: \quad a_i \to a_i w_i \tag{3.2}$$

on an n-letter alphabet $\mathcal{A} = \{a_1, \ldots, a_n\}$. Here, the w_i are n arbitrary words of finite length in the alphabet $\mathcal{A}$. Indeed, for the case of *aperiodic two-letter* substitution chains, this form imposes no restriction at all, since these can all be generated by substitution rules of the form (3.2). To see this, note that any two-letter substitution rule $\bar{\varrho}$ can be transformed appropriately by inner automorphisms, i.e., by replacing $\bar{\varrho} \rightsquigarrow \varrho : a_i \to$

[1] It can be represented in the block-form $\mathcal{H} = \begin{pmatrix} 0 & A \\ A & 0 \end{pmatrix}$ after an appropriate reordering of the basis.

$\hat{w}^{-1}\bar{\varrho}(a_i)\hat{w}$ [where a natural choice of the word $\hat{w}$ is the common beginning, if any, of the words $\bar{\varrho}(a_1)$ and $\bar{\varrho}(a_2)$], and/or by considering $\bar{\varrho}^2$ instead. Obviously, this does not alter the limit chain. Note that this is not possible for certain *periodic* chains, namely those which are generated by a substitution rule that replaces all letters by the same word (the period), or by a multiple of it. It is no problem, however, to treat this case separately.

The eigenvalue problem for the matrix $\mathcal{H}$ (3.1) can be reformulated using transfer matrices in the usual way. Our renormalization transformation (RT) is, however, most conveniently described in terms of the star-product formalism, borrowed from scattering theory [22]. We therefore introduce new S-transfer matrices, called S-matrices from now on, by

$$\begin{pmatrix} \psi_{2j} \\ \psi_{2k+1} \end{pmatrix} = \mathcal{S}_{j|k} \begin{pmatrix} \psi_{2j+1} \\ \psi_{2k} \end{pmatrix} \tag{3.3}$$

with

$$\mathcal{S}_{j|k} = \mathcal{S}_{j|j+1} * \mathcal{S}_{j+1|j+2} * \ldots * \mathcal{S}_{k-1|k} = \mathop{\ast}_{\ell=j}^{k-1} \mathcal{S}_{\ell|\ell+1} \ , \tag{3.4}$$

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

$$\begin{pmatrix} e & \bar{e} \\ r & \rho \end{pmatrix} * \begin{pmatrix} \rho_1 & r_1 \\ \bar{o} & o \end{pmatrix} = \begin{pmatrix} e & 0 \\ 0 & o \end{pmatrix} + \frac{1}{1-\rho\rho_1} \begin{pmatrix} \bar{e}r\rho_1 & \bar{e}r_1 \\ \bar{o}r & \bar{o}r_1\rho \end{pmatrix} \ . \tag{3.5}$$

In our case, according to Eq. (3.1), the elementary S-matrices are

$$\mathcal{S}_{j|j+1} = \begin{pmatrix} \varepsilon_j^{-1}\Lambda & -\varepsilon_j^{-1}h \\ -\varepsilon_{j+1}^{-1}h & \varepsilon_{j+1}^{-1}\Lambda \end{pmatrix} \ , \tag{3.6}$$

where Λ denotes an eigenvalue[2] of $\mathcal{H}$.

In order to establish the renormalization scheme, we introduce a number of additional parameters for these S-matrices. For each letter $a_i \in \mathcal{A}$, we define two asymmetry-coefficients $\kappa_{a_i}^{\pm}$ and a field variable h_{a_i} that enter the n^2 different elementary S-matrices through[3]

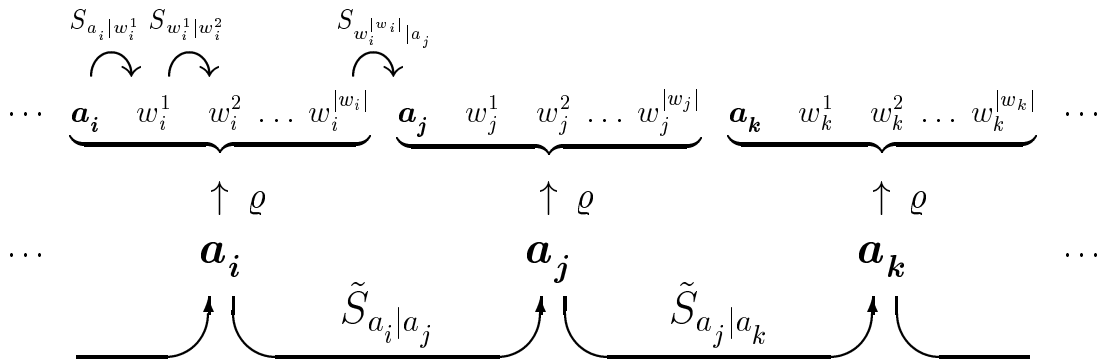
$$S_{a_i|a_j} = \begin{pmatrix} \varepsilon_{a_i}^{-1}\kappa_{a_i}^{+}\Lambda & -\varepsilon_{a_i}^{-1}h_{a_i} \\ -\varepsilon_{a_j}^{-1}h_{a_i} & \varepsilon_{a_j}^{-1}\kappa_{a_i}^{-}\Lambda \end{pmatrix} \ . \tag{3.7}$$

The RT now just *reverses* the substitution steps. In our framework, this is simply done by building $*$-products of the S-transfer matrices that correspond to the words w_i given

[2]So far, we do not have to impose any restriction here, thus Λ may be *any* eigenvalue of $\mathcal{H}$. Only later, after expanding the renormalization equations in powers of Λ [Eq. (3.15) and below], we shall restrict ourselves to eigenvalues that vanish in the limit of an infinite system size.

[3]Note that this labeling of the fields differs from that used in Eqs. (2.1) and (3.1) in that the field variables are now labeled in the same way as the coupling constants (i.e., as the bonds) rather then by the sites of the chain.

by the substitution rule (3.2). Schematically, this works in the following fashion



where w_i^k denotes the kth letter of the word w_i. In this way, we obtain renormalized S-matrices

$$\tilde{\mathcal{S}}_{a_i|a_j} = S_{a_i|w_i^1} * S_{w_i^1|w_i^2} * \cdots * S_{w_i^{|w_i|}|a_j} =: \begin{pmatrix} \varepsilon_{a_i}^{-1}\tilde{\kappa}_{a_i}^{+}\tilde{\Lambda} & -\varepsilon_{a_i}^{-1}\tilde{h}_{a_i} \\ -\varepsilon_{a_j}^{-1}\tilde{h}_{a_i} & \varepsilon_{a_j}^{-1}\tilde{\kappa}_{a_i}^{-}\tilde{\Lambda} \end{pmatrix} , \tag{3.8}$$

compare Eq. (3.6). As an *additional condition* on the RT, and in accordance with their initial values, we keep the product of the $2n$ asymmetry-coefficients $\kappa_{a_i}^{\pm}$ fixed:

$$\prod_{i=1}^{n} \tilde{\kappa}_{a_i}^{+}\tilde{\kappa}_{a_i}^{-} = \prod_{i=1}^{n} \kappa_{a_i}^{+}\kappa_{a_i}^{-} = 1 . \tag{3.9}$$

Now, the RT for the different parameters can be read off directly from the $*$-product relations. Explicitly, we obtain the following recursion relations

$$h_{a_i}^{(1)} = h_{a_i} , \qquad h_{a_i}^{(k+1)} = \frac{-\varepsilon_{w_i^k} h_{w_i^k} h_{a_i}^{(k)}}{\varepsilon_{w_i^k}^2 - \Lambda_{w_i^k+}\Lambda_{a_i-}^{(k)}} , \qquad \tilde{h}_{a_i} = h_{a_i}^{(|w_i|+1)} ; \tag{3.10}$$

$$\Lambda_{a_i-}^{(1)} = \Lambda_{a_i-} , \qquad \Lambda_{a_i-}^{(k+1)} = \Lambda_{w_i^k-} + \frac{h_{w_i^k}^2 \Lambda_{a_i-}^{(k)}}{\varepsilon_{w_i^k}^2 - \Lambda_{w_i^k+}\Lambda_{a_i-}^{(k)}} , \qquad \tilde{\Lambda}_{a_i-} = \Lambda_{a_i-}^{(|w_i|+1)} ; \tag{3.11}$$

$$\Lambda_{a_i+}^{(1)} = \Lambda_{a_i+} , \qquad \Lambda_{a_i+}^{(k+1)} = \Lambda_{a_i+}^{(k)} + \frac{\Lambda_{w_i^k+}\left[h_{a_i}^{(k)}\right]^2}{\varepsilon_{w_i^k}^2 - \Lambda_{w_i^k+}\Lambda_{a_i-}^{(k)}} , \qquad \tilde{\Lambda}_{a_i+} = \Lambda_{a_i+}^{(|w_i|+1)} ; \tag{3.12}$$

for the field variables h_{a_i} and for $\Lambda_{a_i\pm}$ that are defined as

$$\Lambda_{a_i\pm} := \kappa_{a_i}^{\pm}\Lambda , \qquad \tilde{\Lambda}_{a_i\pm} := \tilde{\kappa}_{a_i}^{\pm}\tilde{\Lambda} . \tag{3.13}$$

Using Eq. (3.9), we obtain the renormalized fermion frequencies $\tilde{\Lambda}$ as

$$\tilde{\Lambda} = \left(\prod_{i=1}^{n} \tilde{\Lambda}_{a_i+}\tilde{\Lambda}_{a_i-} \right)^{\frac{1}{2n}} . \tag{3.14}$$

Note the following properties of our renormalization approach:

- The RT is *exact*, since no new parameters are introduced in a renormalization step. Altogether, there are $3n$ parameters for n different couplings: Effectively $2n-1$ asymmetry-parameters $\kappa_{a_i}^{\pm}$, the n fields h_{a_i}, and the eigenvalue Λ. Note that *the coupling constants are not renormalized* in our scheme.

- The rescaling factor of the system size is just given by the leading eigenvalue λ_{PF} of the substitution matrix corresponding to the substitution rule under consideration.

- The critical point of the model, defined by the vanishing of the mass gap ($\Lambda \equiv 0$), corresponds to a fixed point of the RT for Λ, as can easily be seen from Eqs. (3.11) and (3.12).

- The scaling behaviour in the vicinity of the critical point is governed by the leading-order term of the RT as $\Lambda \to 0$.

We now proceed to establish the RT of the spectrum to leading order for $\Lambda \to 0$ explicitly. This is most easily done by noting that, in the product (3.8), the common prefactors $(1-\rho\rho_1)^{-1} = 1 + \mathcal{O}(\Lambda^2)$ of the $*$-products (3.5) gives rise to higher-order corrections only; and therefore, for the present purpose, the denominator can be neglected completely. Consider first the renormalization of the field variables. We obtain

$$\tilde{h}_{a_i} = h_{a_i} \cdot \prod_{\ell=1}^{|w_i|} \frac{-h_{w_i^\ell}}{\varepsilon_{w_i^\ell}} + \mathcal{O}(\Lambda^2) \; . \tag{3.15}$$

Instead of working directly with the RT for the fields, it is advantageous to consider new variables

$$y_i := \log\left(\frac{h_{a_i}^2}{\varepsilon_{a_i}^2}\right) \; . \tag{3.16}$$

To linear order in Λ, the RT of y_i then yields the simple matrix form

$$\tilde{\boldsymbol{y}} = \boldsymbol{M}_\varrho^t \, \boldsymbol{y} \; , \tag{3.17}$$

where $\boldsymbol{M}_\varrho^t$ is just the *transpose* of the substitution matrix of ϱ. Now, take a look at the initial conditions $\boldsymbol{y}^{[0]}$ for $\boldsymbol{y}$ which are $y_i^{[0]} = -2\log\varepsilon_{a_i}$. As stated above, the entries of the (statistically normalized) Perron-Frobenius eigenvector $\boldsymbol{v}_{\mathrm{PF}}$ are the asymptotic letter frequencies $p_i := p_{a_i}$. We thus obtain

$$\boldsymbol{y}^0 \cdot \boldsymbol{v}_{\mathrm{PF}} = -2\log\left[\prod_{i=1}^{n} \varepsilon_{a_i}^{p_i}\right] = 0 \tag{3.18}$$

for an *arbitrary* set of couplings fulfilling the criticality condition (2.5). Hence, $\boldsymbol{y}^{[0]}$ is nothing but an arbitrary (real) linear combination of the (right) eigenvectors of $\boldsymbol{M}_\varrho^t$ (hence

of the *left* eigenvectors of $\boldsymbol{M}_\varrho$) *excluding* the Perron-Frobenius one. Thus, for a generic choice of critical couplings, it scales with the second-largest eigenvalue, $\|\boldsymbol{y}^{[k]}\| \sim |\lambda_2|^k$, under the iteration $\boldsymbol{y}^{[k+1]} = \boldsymbol{M}_\varrho^t \boldsymbol{y}^{[k]}$. Translated into the terminology of the renormalization group, we recognise $\boldsymbol{y}$ as a *scaling field* transforming according to

$$\tilde{\boldsymbol{y}} = (\lambda_{\mathrm{PF}})^\beta \boldsymbol{y} \tag{3.19}$$

where the corresponding *renormalization group eigenvalue* is just the wandering exponent β defined in Eq. (2.9). This demonstrates explicitly that power law, logarithmic, or bounded fluctuations lead to relevant, marginal, or irrelevant scaling fields, respectively. We are going to describe below how this affects the critical behaviour.

We now proceed to the RT for $\Lambda_{a_i\pm}$. Defining

$$P^+_{a_i a_j} := \sum_{k=1}^{|w_i|} \delta_{w_i^k, a_j} \frac{h_{a_i}^2}{h_{w_i^k}^2} \prod_{\ell=1}^{k} \frac{h_{w_i^\ell}^2}{\varepsilon_{w_i^\ell}^2} + \delta_{a_i,a_j} \ , \tag{3.20}$$

$$P^-_{a_i a_j} := \left[\sum_{k=1}^{|w_i|} \delta_{w_i^k, a_j} \prod_{\ell=1}^{k} \frac{\varepsilon_{w_i^\ell}^2}{h_{w_i^\ell}^2} + \delta_{a_i,a_j} \right] \prod_{\ell=1}^{|w_i|} \frac{h_{w_i^\ell}^2}{\varepsilon_{w_i^\ell}^2} \ , \tag{3.21}$$

we find, by induction, as the linear part of the RT of $\Lambda_{a_i\pm}$

$$\tilde{\Lambda}_{a_i\pm} = \sum_{j=1}^{n} \Lambda_{a_j\pm} P^\pm_{a_i a_j} \ . \tag{3.22}$$

Setting $M^\pm_{ij} := P^\pm_{a_i a_j}$, this can also be written in a matrix form

$$\tilde{\boldsymbol{\Lambda}}_\pm = \boldsymbol{M}^\pm \boldsymbol{\Lambda}_\pm \ . \tag{3.23}$$

Since all the components of the matrices $\boldsymbol{M}^\pm$ and of the vectors $\boldsymbol{\Lambda}_\pm$ are positive, the vectors converge to the Perron-Frobenius eigenvectors of $\boldsymbol{M}^\pm$ under iteration of the RT. Let $\mu^\pm$ denote the Perron-Frobenius eigenvalues of $\boldsymbol{M}^\pm$. From Eq. (3.14), we conclude that

$$\tilde{\Lambda}^2 = \mu^+ \mu^- \Lambda^2 \ . \tag{3.24}$$

For further convenience, we transform $\boldsymbol{M}^+$ (under conservation of the spectrum) according to $\boldsymbol{M}^+_T = \boldsymbol{T}^{-1} \boldsymbol{M}^+ \boldsymbol{T}$ with a diagonal transformation matrix $T_{ij} = h_{a_i}^2 \delta_{ij}$. As new entries, we find, dropping the index T,

$$M^+_{ij} = P^+_{a_i a_j} = \sum_{k=1}^{|w_i|} \delta_{w_i^k, a_j} \prod_{\ell=1}^{k} \frac{h_{w_i^\ell}^2}{\varepsilon_{w_i^\ell}^2} + \delta_{a_i,a_j} \ . \tag{3.25}$$

This form shows explicitly that, to linear order in Λ, only the *reduced couplings* $\varepsilon_{a_i}/h_{a_i}$ enter in the RT. Finally, since the rescaling factor of the chain length is the largest

eigenvalue $\lambda_{\rm PF}$ of the substitution matrix, we formally obtain the scaling exponent z through

$$\Lambda_j = x_j N^{-z} \ , \qquad z = \frac{\log\left(\mu^+\mu^-\right)}{2\,\log\left(\lambda_{\rm PF}\right)} \ . \tag{3.26}$$

Let us now look at the different cases of fluctuation behaviour in more detail.

3.1 Bounded Fluctuations

Because $\boldsymbol{y}$ is perpendicular to the Perron-Frobenius eigenvector of the substitution matrix, and since all other eigenvalues are smaller than one in modulus, we find $\|\boldsymbol{y}^{[k]}\| \to 0$ for all substitution chains with bounded fluctuations, hence $h_{a_i}^2/\varepsilon_{a_i}^2 \to 1$. Evaluating the transformation matrices $\boldsymbol{M}^{\pm}$ at this fixed point of the fields, we obtain from Eqs. (3.21) and (3.25)

$$\boldsymbol{M}^+ = \boldsymbol{M}^- = \boldsymbol{M}_\varrho^t \tag{3.27}$$

and hence

$$\mu^+ = \mu^- = \lambda_{\rm PF} \ . \tag{3.28}$$

Thus we have $z = 1$ for substitution chains with bounded fluctuations, and the low-energy spectrum at criticality scales as

$$\Lambda_j = x_j \frac{v}{N} \, . \tag{3.29}$$

Hereby, the Λ-transformation induces a finite renormalization of the *fermion velocity* v in comparison to the uniform chain

$$v = \lim_{\substack{k\to\infty \\ \Lambda\to 0}} \frac{(\lambda_{\rm PF})^k}{\Lambda^{[k]}/\Lambda} \tag{3.30}$$

where $\Lambda^{[k]}$ is the image of $\Lambda^{[0]} = \Lambda$ after a k-fold application of the RT.

In general, all renormalization steps contribute in Eq. (3.30). However, if *all* eigenvalues of the substitution matrix but the Perron-Frobenius one are zero, the fixed point of the RT is already reached after the first renormalization step and v is obtained immediately. This is shown below for periodic chains, but also allows to calculate the fermion velocity of the Thue-Morse and related chains. Using the equidistribution property of quasiperiodic *cut-and-project* chains, like our first example (2.7) with $k = 1$ (the Fibonacci sequence), the limit in Eq. (3.30) can be carried through explicitly for these cases, too. Since this has already been done in Ref. [18], we do not repeat the arguments here, and merely cite the result

$$v(r) = \frac{2\log(r)}{|r - r^{-1}|} \tag{3.31}$$

for two couplings parametrised as in Eq. (2.6).

Periodic chains

In this short part, we briefly show how the known results for the fermion velocity v for *periodic* quantum chains can be recovered easily within our renormalization scheme. By a substitution rule of the form

$$\varrho: \quad a_i \to w \ , \tag{3.32}$$

any periodic chain with period $m = |w|$ can be generated. In this simple situation, we can take all the fields $h_{a_i} \equiv h$ and asymmetry-parameters $\kappa^+_{a_i} \equiv \kappa \equiv (\kappa^-_{a_i})^{-1}$ to be equal. By virtue of the criticality condition (2.5), the reduced couplings transform as $h^2/\varepsilon_i^2 \to 1$ [see Eq. (3.15)], and we obtain the (fermionic) Hamiltonian of a *uniform* chain ($\varepsilon = h = \varepsilon_{w^1}$) after a single renormalization step. Note that the additional asymmetry-parameters result in an irrelevant similarity transformation of the matrix (3.1) only. The renormalization factor for Λ can be deduced from Eqs. (3.21) and (3.25), explicitly it reads (using Eq. (2.5), and normalizing to $\varepsilon = h = 1$):

$$\begin{aligned} m^2 v^{-2} := \frac{\tilde{\Lambda}^2}{\varepsilon_1^2 \Lambda^2} &= \left(1 + \sum_{k=2}^{|w|} \varepsilon_2^2 \cdots \varepsilon_k^2\right) \left(1 + \sum_{k=2}^{|w|} \varepsilon_2^{-2} \cdots \varepsilon_k^{-2}\right) \\ &= \sum_{k=1}^{|w|} \sum_{l=1}^{|w|} \varepsilon_k^2 \cdots \varepsilon^2_{k+l-1(\mathrm{mod}\,|w|)} \end{aligned} \tag{3.33}$$

with $\varepsilon_\ell := \varepsilon_{w^\ell}$. The critical scaling of the fermion frequencies now results in

$$\Lambda_j = \frac{2\pi j}{N} v \ , \qquad j \ll N \ , \tag{3.34}$$

where v is given in Eq. (3.33), and where the well-known scaling behaviour of the uniform chain is recovered for $v = 1$. This result was first derived in the context of the $2d$ classical Ising model with layered periodicity in Ref. [1].

In general, there is no closed expression for the fermion velocity v. For the special case of a uniform chain of ε_a-couplings with periodic ε_b-defects on every mth site, we derive

$$v(r) = \frac{\sinh[\log(r)/m]}{\sinh[\log(r)]/m} \ . \tag{3.35}$$

Note that $v(r) = 1$ for $m = 1$ (simple periodic chain), but also $v(r) \to 1$ for $m \to \infty$ since the parametrisation (2.6) implies that $r \to 1$ in this limit.

3.2 Marginal fluctuations

We now consider the case where the second-largest eigenvalue(s) of the substitution matrix (and of its transpose) have $|\lambda| = 1$. Let E_1 denote the corresponding m-dimensional

(joined) eigenspace of $\boldsymbol{M}_\varrho^t$, where $1 \leq m \leq n-1$. By Eqs. (3.17) and (3.18), $\boldsymbol{y}^{[k]}$ converges to the projection of $\boldsymbol{y}^{[0]}$ on E_1 under iteration of the RT. The critical surface being $(m-1)$-dimensional, we can parametrise $\boldsymbol{y} = \boldsymbol{y}^{[\infty]}$ in the renormalization limit as

$$\boldsymbol{y} = \sum_{i=1}^{m} \log(r_i)\, \boldsymbol{v}^i \tag{3.36}$$

with m vectors $\boldsymbol{v}^i$ that span E_1 and coefficients $r_i > 0$, $i = 1, 2, \ldots, m$. This implies

$$\frac{h_{a_j}^2}{\varepsilon_{a_j}^2} = \exp(y_j) = \prod_{i=1}^{m} r_i^{v_j^i} \tag{3.37}$$

and, if the vector components v_j^i are chosen as integers, the entries of the matrices $\boldsymbol{M}^\pm$ are polynomials with positive coefficients of m parameters $r_1^{\pm 1}, \ldots, r_m^{\pm 1}$. If all r_i are equal to 1, we obviously obtain

$$\boldsymbol{M}^+(r_i{=}1) = \boldsymbol{M}^-(r_i{=}1) = \boldsymbol{M}_\varrho\ . \tag{3.38}$$

Furthermore, if $\boldsymbol{y}^{[k]}$ converges to an eigenvector of $\boldsymbol{M}_\varrho^t$ to the eigenvalue $\lambda_2 = 1$, $\boldsymbol{M}^+$ and $\boldsymbol{M}^-$ are related by

$$M_{ij}^+(r_1, \ldots, r_m) = M_{ij}^-(r_1^{-1}, \ldots, r_m^{-1})\ . \tag{3.39}$$

To obtain the scaling exponent z from Eq. (3.26), we need to know the Perron-Frobenius eigenvalues $\mu^\pm$ of $\boldsymbol{M}^\pm$. There is no explicit solution to that problem in the general case. In what follows, we present the complete answers for a number of more special, yet infinite, classes of substitution rules.

Cyclic permutations

Let w be any word from the alphabet, and $p_k(w)$ its kth cyclic permutation. Consider now a substitution rule ϱ of the form (3.2) with

$$w_i = [p_{k_i}(w)]^{l_i}\ . \tag{3.40}$$

One special case is to take equal words $w_i = w$ for all $i = 1, 2, \ldots, n$. The corresponding substitution matrices indeed have $\lambda_2 = 1$ as their second-largest eigenvalue, with degeneracy $(n-1)$, since the column vectors of $\boldsymbol{M}_\varrho - \mathbb{I}$ differ by scalar factors only. Thus the fields stay at their original values and are not renormalized at all. To derive $\mu^\pm$ as a function of the parameters $r_1, \ldots, r_{n-1}$, we simply note that the special form of ϱ transforms this property to $\boldsymbol{M}^\pm$, not just for the point $r_i = 1$, $\forall i$, but *independently* of the parameters. We thus obtain

$$\mu^\pm = \mathrm{tr}(\boldsymbol{M}^\pm) - n + 1 > 1 \tag{3.41}$$

and the scaling exponent is given by

$$z = \frac{\log\left(1 - n + \sum_{i=1}^{n} P^{+}_{a_i a_i}\right) + \log\left(1 - n + \sum_{i=1}^{n} P^{-}_{a_i a_i}\right)}{2\log(\lambda_{\mathrm{PF}})} \,, \tag{3.42}$$

where the $P^{\pm}_{a_i,a_j}$ are given in Eqs. (3.21) and (3.25) as functions of the couplings. Since $\mu^{\pm}$ are polynomials of the parameters $r_i^{\pm 1}$ with only positive coefficients, and $\mu^{+}(\{r_i\}) = \mu^{-}(\{r_i^{-1}\})$, we conclude $z \geq 1$. As a function of the parameters, z is either purely *convex*, with unique minimum $z(r_i = 1) = 1$ (the limit of the uniform chain), or it is *constant*: $z \equiv 1$. It is interesting to take a closer look at the latter case. Obviously, this means that $P^{\pm}_{a_i a_i} = [\boldsymbol{M}_{\varrho}]_{ii}$, independently of the parameters. As can be shown, for substitution rules of the form (3.2) with (3.40), this is possible if and only if w is a word (or a power of a word) with all letters a_i appearing precisely once and if the last letter of w_i is a_i. This means, however, that the resulting chain is *periodic* and has bounded rather than logarithmically diverging fluctuations.

Two-letter substitution rules

As stated above, each two-letter substitution chain can be generated by a substitution rule of the form (3.2). For any marginal substitution rule, we can assume that the second-largest eigenvalue of the substitution matrix is $\lambda_2 = +1$. If necessary, this can be achieved by going to ϱ^2. As a consequence, $\boldsymbol{y}^{[0]}$ in Eq. (3.17) is eigenvector to the eigenvalue $\lambda_2 = 1$ of $\boldsymbol{M}^{t}_{\varrho}$, and as above the fields are already at their fixed points.

In this case, the entries of the transformation matrices $\boldsymbol{M}^{\pm}$ are polynomials of a single parameter r that determines the critical couplings. The crucial point now is to show that – like in the case discussed above – the matrices $\boldsymbol{M}^{\pm}$ have an eigenvalue $\lambda_2 = 1$ independently of r and of the detailed form of the substitution rule. This assertion is proved in Appendix A. Then, the Perron-Frobenius eigenvalues of $\boldsymbol{M}^{\pm}$ are given as above (3.41), and we obtain the critical scaling exponent

$$z(r) = \frac{\log(P^{+}_{aa} + P^{+}_{bb} - 1) + \log(P^{-}_{aa} + P^{-}_{bb} - 1)}{2\log(\lambda_{\mathrm{PF}})} \tag{3.43}$$

where λ_{PF} is the leading eigenvalue of the substitution matrix. As in the case discussed above, $z(r)$ is constant ($z \equiv 1$) only for the special case of a periodic chain (with period ab). Otherwise, z is a convex function of r, with a unique minimum $z(1) = 1$ where the (reduced) couplings are equal. On the other hand, it is easy to see that the periodic chain with period ab is the only two-letter substitution chain with bounded letter fluctuations that can be generated by a substitution rule of the form (3.2) and that has $\lambda_2 = 1$ as the second-largest eigenvalue of the substitution matrix. We thus conclude that $z \equiv 1$ *if and only if* the fluctuations are bounded, and $z > 1$ otherwise.

Examples

The *period-doubling chain*, given by the substitution rule (2.7) with $k = 2$, falls into both classes described above. We consider double substitution steps, eliminating blocks of the form *aba* and obtain the scaling exponent

$$z(r) = \frac{\log(r^{1/3} + r^{-1/3})}{\log(2)} \tag{3.44}$$

This result was reported before in Ref. [15]. If the length of the chain is increased by simple substitution steps, the coefficients x_j in Eq. (3.26) converge *separately* for an even and an odd number of steps. Effectively, this can be seen as a renormalization of the couplings according to $r = \varepsilon_a/\varepsilon_b \to r^{-1}$ in a single renormalization step. Hence we obtain $x_j^{\mathrm{odd}}(r) = x_j^{\mathrm{even}}(r^{-1})$.

As an example that is not contained in the above classes, consider the three-letter substitution

$$\varrho: \begin{array}{rcl} a & \to & abc \\ b & \to & ba \\ c & \to & ca \end{array} \tag{3.45}$$

with eigenvalues of the substitution matrix $\lambda_{1,3} = 1 \pm \sqrt{2}$ and $\lambda_2 = 1$. The eigenvector to eigenvalue 1 of the transposed substitution matrix $\boldsymbol{M}_\varrho^t$ is $(0, t, -t)$, and with Eq. (3.16) we conclude that $h_a^2 \to \varepsilon_a^2$ and $h_{b,c}^2 \to \varepsilon_b\varepsilon_c$. Evaluating the RT of $\boldsymbol{\Lambda}_\pm$ at this fixed point, we obtain the critical scaling exponent

$$z = \frac{\log\left(1 + \sqrt{1 + \varepsilon_c/\varepsilon_b}\right) + \log\left(1 + \sqrt{1 + \varepsilon_b/\varepsilon_c}\right)}{2\,\log(1 + \sqrt{2})} \tag{3.46}$$

Note that, for $\varepsilon_b = \varepsilon_c$, the fluctuations of the couplings are indeed bounded, and we obtain $z = 1$ as it should be. In our last example, the couplings follow the Thue-Morse sequence on the *sites* of the chain, rather than on the bonds as in all cases discussed so far. The coupling constants for a site-problem are given as a function of the two adjacent bonds – and thus can take in general n^2 different values ($2^2 = 4$ in this case). It can, however, easily be shown that this can be reformulated as a bond-problem with a substitution chain on an n^2-letter alphabet [21, 4, 25]. In this case, the resulting four-letter substitution rule is

$$\varrho: \begin{array}{rcl} a & \to & acdb \\ b & \to & bcdb \\ c & \to & cbac \\ d & \to & dbac \end{array} . \tag{3.47}$$

The asymptotic letter frequencies are $p_a = p_d = 1/6$ and $p_b = p_c = 1/3$; and so we have $\varepsilon_a\varepsilon_d\varepsilon_b^2\varepsilon_c^2 = 1$ (for $h = 1$) as the criticality condition (2.5). A possible parametrisation

is $\varepsilon_a = q^2$, $\varepsilon_d = r^2$, $\varepsilon_b = s$, and $\varepsilon_c = (qrs)^{-1}$. The eigenvalues of the substitution matrix are 4, 1, 1, and 0, we thus expect marginal fluctuations, whereas the Thue-Morse bond-problem has bounded fluctuations. Following the above steps, we obtain a scaling exponent

$$z = \frac{\log\left[(qr)^{1/4} + (qr)^{-1/4}\right]}{\log(2)} \; . \tag{3.48}$$

Note that for $\varepsilon_a = \varepsilon_d$, $\varepsilon_b = \varepsilon_c$ we obtain another coding of the period-doubling chain, while the special case $\varepsilon_a = \varepsilon_b$, $\varepsilon_c = \varepsilon_d$ leads us back to the Thue-Morse bond-problem with bounded fluctuations (with $q = r^{-1}$, and thus $z = 1$).

3.3 Relevant fluctuations

For $|\lambda_2| > 1$, fluctuations diverge with a power law. As a consequence, the vector $\boldsymbol{y}^{[k]}$ finally scales with $|\lambda_2|$ under the RT. Since the matrix elements of $\boldsymbol{M}^{\pm}$ are proportional to $\exp(y_i)$, at least a part of them eventually diverge like $\exp(c|\lambda_2|)$ [note that the components of $\boldsymbol{y}$ have different sign because of Eq. (3.18)]. Estimating the product of the Perron-Frobenius eigenvalues $\mu^{\pm}$ by the product of the corresponding traces, we obtain

$$\tilde{\Lambda}^2 \sim \tilde{\mu}^+ \tilde{\mu}^- \sim \Lambda^{2|\lambda_2|} \tag{3.49}$$

and thus

$$\Lambda \sim \exp\left(-cN^{\beta}\right) \tag{3.50}$$

where the *wandering exponent* β is defined in Eq. (2.9).

Two-letter substitutions

Let us discuss this in more detail for the case of two-letter substitutions. We take $\lambda_2 > 1$ with corresponding eigenvector $\boldsymbol{v}$ of $\boldsymbol{M}^t_{\varrho}$ and parametrise the critical couplings as

$$\frac{h^2_{a,b}}{\varepsilon^2_{a,b}} = r^{v_{a,b}} \; . \tag{3.51}$$

Since v_a and v_b have different sign, either one of these two is bigger than one for a fixed value $r \neq 1$, and without loss of generality we assume $r^{v_a} > 1$. Note that we have the following relation

$$\prod_{\ell=1}^{|w_a|} \frac{h^2_{w_a^\ell}}{\varepsilon^2_{w_a^\ell}} = r^{(\lambda_2 - 1)v_a} \; . \tag{3.52}$$

We now show that $P^{\pm}_{aa} \geq \exp\left[(\lambda_2 - 1)v_a \log r\right]$. From Eq. (3.21), this is immediately clear for P^{-}_{aa}, but it also holds for P^{+}_{aa}. To see this, consider the products of subsequent couplings of the word w_a. The product of the entire word is given by Eq. (3.52). If the

last letter of w_a is an a, this enters P^+_{aa} and we are done. On the other hand, if the last letter is a b, consider the product of all couplings but the last h_b^2/ε_b^2, which is even larger. Iterating this argument, we finally arrive at a letter a which proves our estimate of P^+_{aa}. Using the standard eigenvalue formula, we obtain the scaling of $\mu^\pm$ under the RT, and thereby

$$\Lambda \sim \exp\left(-c|\log r|\, N^\beta\right) \ . \tag{3.53}$$

Here, c is some constant that may depends on the sign of $\log(r)$, but apart from that is independent of r and N. This scaling form was also predicted in [18].

4 Scaling behaviour and critical properties

In this section, we give a short summary of the results of our renormalization treatment and discuss their consequences for the critical properties of the IQC.

4.1 Results: Bounded fluctuations

Here, the behaviour of the low-energy part of the the spectrum at criticality is essentially the same as for the uniform chain. The correlation length critical exponents stays at its Onsager value $z = \nu_\parallel = \nu_\perp = 1$. For periodic chains (or periodic variations of the interactions along the layers of the $2d$ statistical system), the results from renormalization show that the smallest fermion frequencies are only altered by a common factor v (fermion velocity), thus also conformal properties persist and the whole model is described by the central charge $c = 1/2$ conformal field theory of a massless free Majorana fermion:

$$\Lambda_j \ \sim \ x_j \, \frac{\pi v}{N} \tag{4.1}$$

with a fermion velocity v given by (3.33).The scaling dimensions x_j are odd integers for periodic boundary conditions (mixed sector Hamiltonian) and odd half-integers for free boundaries [8]. Numerical results [12] confirm this conformal behaviour even for non-periodic chains with bounded fluctuations.

4.2 Results: Logarithmically diverging fluctuations

For the critical scaling, we can make the following *Ansatz*:

$$\Lambda_j \ = \left(\frac{j}{N}\right)^{z(r)} F_r(j,N) \tag{4.2}$$

The index r here denotes the dependence on the position on the critical surface. The predicted scaling behaviour [18] is confirmed analytically for all marginal two-letter substitution chains and some infinite classes of n-letter substitution chains. $j^z F_r(j,N)$ converges to the scaling coefficients x_j if we increase the length of the chain N by (multiple)

substitution steps, in other words $F_r(j, \log N)$ is asymptotically periodic for $N \gg 0$ with period $\log \lambda_{\rm PF}$, where $\lambda_{\rm PF}$ is the scaling factor of the system size. Eq. (3.43) implies $1 \leq z < \infty$, and $z = 1$ is only obtained in the limit of the uniform chain where the fluctuations actually vanish. We further note that, in the explicitly solved cases, z is invariant under inversion of all couplings. Thus this is a symmetry of the lower part of the critical spectrum, while it is easy to see that it is not a symmetry of the entire finite-size spectrum. As a consequence, z quadratically approaches the isotropic value $z_0 = 1$ for small deviations of the couplings from the uniform strength $\varepsilon_\alpha = 1$, as was also predicted by Luck [18].

In the terminology of the $2d$ classical Ising model, we have $\nu_\parallel = z > 1$ for any marginal disorder within layers of couplings. Since the correlation length critical exponent perpendicular to the layers remains $\nu_\perp = 1$, marginal fluctuations introduce a relevant anisotropy of the model, as was noticed in Ref. [6]. Due to anisotropic hyperscaling, a *negative* specific heat exponent

$$\alpha = 2 - \nu_\parallel - \nu_\perp = 1 - z \tag{4.3}$$

is expected.

Within the renormalization approach, the length of the chain N is increased by (multiple) substitution steps. Thus, it is a priori not clear what happens to the scaling dimensions when we increase N arbitrarily. Indeed, numerical studies (for free boundary conditions) show that, if we increase N by arbitrary amounts, while z converges, $F_r(j, N)$ stays finite but will not tend to a unique limit. This is in contrast to the bounded fluctuation case. In more detail, the following properties of $F_r(j, N)$ have been observed in all examples (of two-letter substitution chains) studied:

- Given the couplings, $F_r(j, N)$ appears to be bounded for all N and j.
- For $N > j \gg 0$, the effect of j on F_r is a mere shift: $F_r(j, N) \sim F(\log(N/j))$.
- As a consequence of the RT, $N \gg j$, $F_r(j, \log N)$ is asymptotically periodic.
- The amplitude of F_r vanishes in the limit of the uniform chain, $r \to 1$, as F_r approaches continuously the constant value π.

These points can immediately be translated into properties of the integrated density of states (IDOS), the inverse of which is given by

$$\sigma^{-1}(\rho) = \rho^z F_r(-\log \rho) \ , \quad 0 < \rho \leq 1. \tag{4.4}$$

While the first two points imply the convergence of this quantity, the third point above implies the lower part of the IDOS to be self-similar with a discrete scaling symmetry

$$m\sigma(\omega) = \sigma(m^z \omega) = \sigma(\omega/v) \ , \sigma(\omega) \sim \omega^{1/z} \tag{4.5}$$

where $\log m$ is the asymptotic period of F_r. Mind that in general not the spectrum (the lowest fermion frequencies), but only the IDOS displays this scaling behaviour for $N \gg 0$.

This scaling property has consequences for the possible gap structure of the critical spectrum, where the results of the renormalization approach at least lead to necessary conditions for gap-labelling theorems. But since within this class more spectral properties can be found analytically using trace maps, we postpone the discussion to a forthcoming publication.

4.3 Results: Relevant fluctuations

In substitution sequences with strong fluctuations, as in our third example, the binary non-Pisot sequence [$k = 3$ in Eq. (2.7)], their divergence is described [18] by the wandering exponent β (2.9) which determines the exponential closing of the spectral gaps as

$$\Lambda_j \;\sim\; \left(A(r) \,+\, B(r)\, N^{-\alpha_j(r)}\right) \,\exp\left(-F_r(j,N)\Delta(r)\,\left(\frac{N}{j}\right)^{\beta}\right) \,. \tag{4.6}$$

Here, $\Delta(r)$ is the mean deviation of the distribution of reduced coupling constants along the chain [18] which for the binary non-Pisot sequence is given by

$$\Delta(r) \;=\; \sqrt{2\sqrt{13}-7} \quad |\log(r)| \;\approx\; 0.459 \;|\log(r)| \tag{4.7}$$

and compatibility with the uniform case requires $A(1) = 0$ and $\alpha_j(1) = 1$.

From the results of the renormalization approach, $F_r(j, \log N)$ should be asymptotically periodic for $N \gg j$. This is confirmed by numerical investigations. Indeed, the latter suggest the very same properties as given above in the case of marginal fluctuations. In particular, we observe $F_r(j,N) = F_r(\log(N/j))$ for $j \gg 0$.

Again, this means that the integrated spectral density converges in the thermodynamic limit and its lower part shows the following scaling property at the critical point:

$$\sigma(\omega^{(m^{-\beta})}) = m\sigma(\omega)\;, \sigma(\omega) \sim (\log\omega)^{-1/\beta}\;, \quad \omega \ll 1\;. \tag{4.8}$$

5 Concluding remarks

Using a renormalization approach, we obtained analytic results for the critical behaviour of a class of Ising models intermediate between uniformly (or periodically) ordered and randomly disordered systems. The systems under consideration are ferromagnetic Ising quantum chains whose interaction constants are modulated according to substitution sequences. Luck's criterion [18] for the relevance of aperiodic disorder on the critical behaviour is fully confirmed for these systems, bringing along increasing evidence that

the *fluctuation of the interactions* is the basic concept that demarcates the Onsager universality class from models with weaker critical singularities. For two-letter substitution rules, this analysis was carried out in detail, showing how the renormalization flow is determined by the nature of the fluctuations. An exact renormalization formalism for the most general case of n-letter substitution rules was also presented and applied to examples.

A number of quantitative results have been displayed, mainly for the correlation length critical exponent (resp. the scaling exponent z of the mass gap), confirming and refining Luck's predictions for bounded, marginal, and relevant fluctuations of the coupling constants. In particular, an exact formula has been obtained for the scaling exponent of arbitrary two-letter substitution chains, containing previous results as special cases. In this light, the case of two-letter substitution rules appears to be rather well understood by now.

What remains to be done in the n-letter case is a thorough discrimination between quantum (substitution) chains with bounded and with marginal fluctuations of the couplings. This is connected with the problem of determining all substitution rules with second-largest eigenvalue of the substitution matrix on the unit circle, which nevertheless result in a chain with bounded rather than marginal fluctuations. Also, the investigation of ordered cases that do not stem from a substitution rule might add some insight as they can possess a higher degree of complexity. Unfortunately, renormalization techniques will probably be unsuitable here.

Of primary interest are, of course, extensions to higher dimensions. A natural first step is to study two-dimensional statistical systems with two-dimensional rather than one-dimensional variations of the interactions. As can be seen from some special cases [3], analytic results are possible in principle, but they are not generic and solvable cases might actually be misleading. Further analysis is necessary, and some results can be expected from numerical approaches, especially since structures generated by substitution rules are well-suited for (numerical) renormalization. First results in this direction have been obtained recently [23] and will be extended soon.

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Appendix A: Solution of the eigenvalue problem for two-letter substitutions

We consider two-letter chains generated by substitution rules

$$\varrho: \quad \begin{array}{ccc} a & \to & aw_a \\ b & \to & bw_b \end{array} \tag{A.1}$$

which have $\lambda_2 = 1$ as the second-largest eigenvalue of the corresponding substitution matrix. As a consequence, one finds the constraints

$$p_a = \frac{\#_a(w_a)}{|w_a|} = \frac{\#_a(w_b)}{|w_b|}\,, \qquad p_b = \frac{\#_b(w_a)}{|w_a|} = \frac{\#_b(w_b)}{|w_b|}\,, \tag{A.2}$$

on the words w_a and w_b and the letter frequencies $p_{a,b}$ in the limit word, where $\#_\alpha(w_\beta)$ denotes the number of letters α contained in the word w_β. We parametrise the criticality condition (2.5) $\varepsilon_a^{p_a}\varepsilon_b^{p_b} = 1$ (setting $h = 1$) for the corresponding Ising chain by

$$\varepsilon_a = r^{-l/2}\,, \quad \varepsilon_b = r^{k/2}\,, \tag{A.3}$$

with *coprime* integers k and l, such that $lp_a = kp_b$. Then $k+l$ divides $|w_a|$ and $|w_b|$.

The scaling exponent of the critical spectrum is a simple expression of the leading eigenvalues of two matrices

$$\boldsymbol{M}^{\pm} = \begin{pmatrix} P^{\pm}_{aa} & P^{\pm}_{ba} \\ P^{\pm}_{ab} & P^{\pm}_{bb} \end{pmatrix} \tag{A.4}$$

where the entries $P^{\pm}_{xy}$ are defined in Eqs. (3.21) and (3.25). They are polynomials in r and r^{-1}. In what follows, we prove that $\boldsymbol{M}^{\pm}$ have an eigenvalue $\lambda_2 = 1$, *independently* of the value of r and of the detailed form of the substitution rule ϱ. Since we have $\boldsymbol{M}^{+}(r) = \boldsymbol{M}^{-}(r^{-1})$, it suffices to concentrate on $\boldsymbol{M}^{+}$.

We define two polynomials $P^{a,b}$ corresponding to the words w_a and w_b by

$$P^a(r, r^{-1}, u) := (P^+_{aa} - 1) + uP^+_{ab}\,, \qquad P^b(r, r^{-1}, u) := P^+_{ba} + u(P^+_{bb} - 1)\,. \tag{A.5}$$

Taking the frequencies $p_{a,b}$ of the letters as given, the possible words w_a and w_b are subject to the constraints (A.2). We define an *elementary polynomial* $P^e(r, r^{-1}, u)$ to be the polynomial $P^{a,b}$ corresponding to a word w_e of minimal length fulfilling this condition. Since k and l are coprime, each w_e consists of k a's and l b's and leads to one of $\binom{k+l}{l}$ different elementary polynomials possible.

Let in the following w be w_a or w_b. We now introduce a graphical representation of the word w and the accompanying polynomials. For given w, construct iteratively a step function $g_w : [0; |w|] \to \mathbb{Z}$ as follows:

$$\begin{aligned} g_w(0) &= 0 \\ g_w(x) &= \left\{ \begin{array}{ll} g_w(k-1) + l & \text{if } w^k = a \\ g_w(k-1) - k & \text{if } w^k = b \end{array} \right\} \quad \text{for } k-1 < x \le k\,. \end{aligned} \tag{A.6}$$

Note that the criticality conditions imply $g_w(|w|) = 0$. An example for the case $k = 2$, $l = 3$ is shown in Figure 1. For $w = w_a$ ($w = w_b$), $P^+_{aa} - 1$ (resp. P^+_{ba}) is given by the "sum

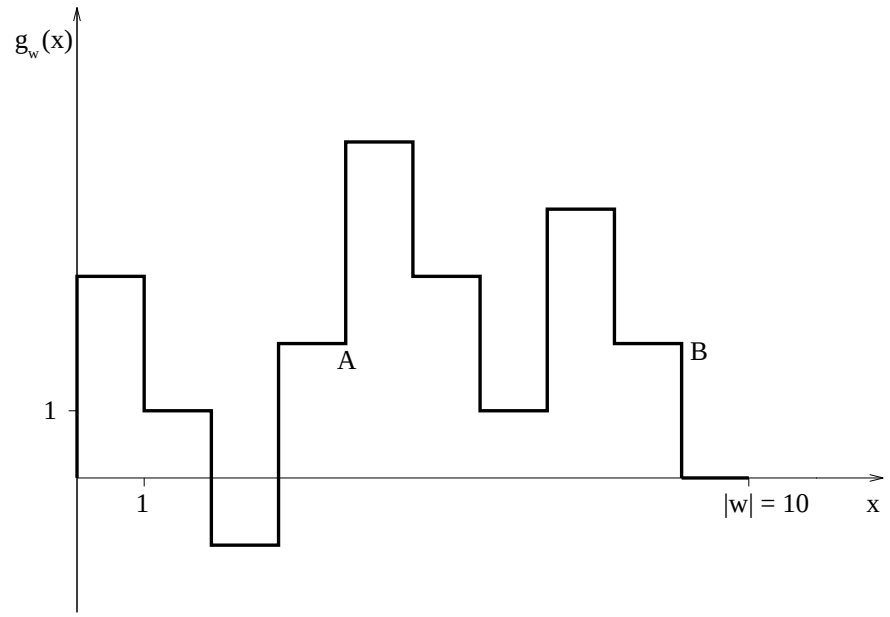

Figure 1: Step function $g_w(x)$ (A.6) of the word $w = abbaabbabb$. The endpoints of an elementary polynomial that can be separated are marked by 'A' and 'B'.

over the *upward* steps" of g_w (proceeding in positive x-direction), while P^+_{ab} (resp. $P^+_{bb} - 1$) is given by the "sum over the *downward* steps", each step contributing a term $r^{g_w(k)}$. In our example (for $w = w_a$), $P^+_{aa} - 1 = r^3 + r^2 + r^5 + r^4$ and $P^+_{ab} = r + r^{-1} + r^3 + r + r^2 + 1$.

In a first step, we now show that $P^{a,b}$ can be expressed as sums over elementary polynomials P^e.

Lemma: For an arbitrary word w fulfilling the criticality condition for given $p_{a,b}$, there are integers a_i and elementary polynomials P^e_i, such that

$$P^{a,b}(r, r^{-1}, u) = \sum_i r^{a_i} P^e_i(r, r^{-1}, u) \tag{A.7}$$

Proof: Consider the substrings s_j of w of length $k + l$ starting with the letter w^j. For each s_j containing more than k a's, there has to be an s_i with less than k a's, because of the criticality condition for w. Since the number of a's contained in successive substrings s_j and s_{j+1} differs at most by one, there is at least one substring consisting of k a's and l b's. In the graphical representation, this appears as a restriction of g_w to an interval of length $k + l$ with the endpoints of the graph taking the same value. The corresponding term within $P^{a,b}$ is obviously some elementary polynomial times a power of r. We may now eliminate this substring from w (cut out the interval in the graphical picture) and start the argument again.

We proceed by showing that the elementary polynomials differ only in a (polynomial) factor that is independent of u.
Proposition: Given k and l, there are polynomials $P_k(r, r^{-1})$ and $P_l(r, r^{-1})$ such that for every elementary polynomial P^e

$$P^e(r, r^{-1}, u) = Q^e(r, r^{-1}) \left[P_k(r, r^{-1}) + u P_l(r, r^{-1}) \right] \tag{A.8}$$

where $Q^e(r, r^{-1})$ is a polynomial that does not depend on u.
Proof: An elementary polynomial P^e takes the following general form

$$P^e = r^{l-c_1 k} + r^{2l-c_2 k} + \ldots + r^{kl-c_k k} + u \left(\sum_{j=1}^{c_1} r^{-jk} + \sum_{j=c_1}^{c_2} r^{l-jk} + \ldots + \sum_{j=c_k}^{l} r^{kl-jk} \right) \tag{A.9}$$

where $0 \leq c_1 \leq c_2 \leq \ldots \leq c_k \leq l$ are integers. Defining

$$P_k := \sum_{j=0}^{k-1} r^j = \frac{1-r^k}{1-r} \; , \quad P_l := \sum_{j=1}^{l} r^{-j} = \frac{r^{-l}-1}{1-r} \; , \tag{A.10}$$

the proof then follows by direct calculation. We remark that with this choice of P_k and P_l, Q^e can also be shown to be a polynomial in r and r^{-1}.

Now, we are in the position to complete our argument. From Eqs. (A.5), (A.7) and (A.8), we conclude that

$$\frac{P_{aa}-1}{P_{ab}} = \frac{P_k}{P_l} = \frac{P_{ba}}{P_{bb}-1} \; . \tag{A.11}$$

Thus it follows that $\det(\boldsymbol{M}^+ - \mathbb{I}) = 0$, and hence $\lambda_2 = 1$ is an eigenvalue of $\boldsymbol{M}^+$ for an *arbitrary* value of r. The leading eigenvalues of $\boldsymbol{M}^{\pm}$ are given by Eq. (3.41).

Appendix B: Renormalization formalism for general n-letter substitution rules

In the above discussion, the coupling constants were chosen according to a substitution rule of the special form (3.2). While any (infinite) substitution chain with two letters can be generated that way, this is no longer the case for three or more different letters (resp. couplings). In this Appendix, we present a generalised version of the renormalization formalism to deal with the general case. Consider a substitution rule of the form

$$\varrho : \;\; a_i \to w_i = w_{i1} a_i w_{i2} \; . \tag{B.1}$$

The main problem in the general case is to maintain the recursive structure of the renormalization procedure within the elimination process. By fixing the first letter of the substitutes in Eq. (3.2), the appropriate couplings of the renormalized chain were given. This is no longer possible here; however, we can proceed as follows.

- Fix any letter a_i within the word $w_i = \varrho(a_i)$, thus defining two words w_{i1} and w_{i2} as shown in Eq. (B.1). Note that the letter a_i appears in the word w_i (at least for a suitably chosen power ϱ^k of the substitution rule) for primitive substitutions.

- Redefine the substitution rule as a function on *pairs* of letters in the following way

$$\varrho \rightsquigarrow \bar{\varrho}: \quad a_i(a_j) \to a_i w_{i2} w_{j1}(a_j) \tag{B.2}$$

  Obviously, (B.2) leads to the same limit chain as (B.1). The substitution matrix of $\bar{\varrho}$ has a dimension of at most n^2 (pairs $a_i a_j$ that do not appear in the original chain need not be included in $\bar{\varrho}$). Actually, $\boldsymbol{M}_{\bar{\varrho}}$ is just the substitution matrix of the corresponding *site*-problem, where the type of site follows the sequence, and the bond (resp. the interaction along it) is a function of its two endpoints [21, 25]. Note, however, that the couplings here are still attached to the bonds.

- In the renormalization formalism, now define S-matrices, fields and asymmetry-parameters corresponding to pairs of letters

$$S_{a_i|a_j} = \begin{pmatrix} \varepsilon_{a_i}^{-1} \kappa^{+}_{a_i a_j} \Lambda & -\varepsilon_{a_i}^{-1} h_{a_i a_j} \\ -\varepsilon_{a_j}^{-1} h_{a_i a_j} & \varepsilon_{a_j}^{-1} \kappa^{-}_{a_i a_j} \Lambda \end{pmatrix} . \tag{B.3}$$

  Renormalization again means inverting the substitution process by integrating out all degrees of freedom attached to the words w_{i1} and w_{i2}. We obtain renormalized S-matrices through

$$\tilde{S}_{a_i|a_j} = S_{a_i|w^1_{i2}} * S_{w^1_{i2}|w^2_{i2}} * \ldots * S_{w^{|w_{i2}|}_{i2}|w^1_{j1}} * \ldots * S_{w^{|w_{j1}|}_{j1}|a_j} . \tag{B.4}$$

- The RT (and their linear orders in Λ) for the (at most) $3n^2$ parameters are then obtained analogous to Section 3.

For a classification of the critical behaviour based on the fluctuations we need to know about the spectrum $\sigma_{\bar{\varrho}}$ of $\boldsymbol{M}_{\bar{\varrho}}$ in dependence of the spectrum σ_{ϱ} of $\boldsymbol{M}_{\varrho}$. For an appropriate power of ϱ, it is indeed possible to show that $\sigma_{\bar{\varrho}}$ contains σ_{ϱ} and that all additional eigenvalues are either 1 or 0. We only sketch the proof here. Without restriction of the general case, we can assume that the first and the last letters of all words w_i remain fixed under the substitution; that is $w_i^1 = [\varrho(w_i)]^1$ for the first letter, and equivalently for the last letter. This is always fulfilled by a finite power ϱ^r of the substitution rule. We assume the n words w_i to have k different first letters and j different last letters. Taking a look at the associated pair substitution matrix $\boldsymbol{M}_{\bar{\varrho}}$, it is easy to show that

$$\mathrm{tr}(\boldsymbol{M}_{\bar{\varrho}}) = \mathrm{tr}(\boldsymbol{M}_{\varrho}) + n + kj - k - j . \tag{B.5}$$

Since we always have $\overline{\varrho^m} = (\bar{\varrho})^m$ and the numbers k and j remain fixed because of the above assumption, the traces of $(\boldsymbol{M}_{\bar{\varrho}})^m$ and $(\boldsymbol{M}_{\varrho})^m$ differ only by the constant $n+kj-k-j$ for arbitrary m. We conclude that $\sigma_{\bar{\varrho}}$ containes σ_{ϱ} and the all additional eigenvalues are fixed points under any power, thus 1 or 0.

We will, however, not give a detailed discussion of the general case here, but rather illustrate the method by applying it to a special example. Consider the substitution rule of the "circle sequence". This example of a quasiperiodic chain (in the sense that it has a pure point Fourier spectrum) has been studied numerically in Ref. [18]

$$\begin{array}{rcccl} & a & \to & cac & \to \quad \underline{a}bcaccacabcac \\ \varrho: & b & \to & accac & \to \quad cacab\underline{b}cacabcaccacabcac \\ & c & \to & abcac & \to \quad \underline{c}acaccacabcaccacabcac \end{array} \tag{B.6}$$

with ϱ^2 being of the form (B.2). The eigenvalues of $\boldsymbol{M}_{\varrho^2}$ are τ^6, 1, and τ^{-6}, where $\tau = (1+\sqrt{5})/2$ is the golden mean – we thus expect marginal fluctuations. The asymptotic frequencies of the letters are $p_a = 2-\tau$, $p_b = \tau - 3/2$, and $p_c = 1/2$, respectively. We choose $\varepsilon_a = rs^{-\tau}$, $\varepsilon_b = rs$, and $\varepsilon_c = r^{-1}s$ as the parametrisation of the critical couplings $\varepsilon_a^{p_a}\varepsilon_b^{p_b}\varepsilon_c^{p_c} = 1$. Since only the five pairs ab, ac, bc, ca, and cc appear in the chain, the dimension of the pair transfer matrix $\boldsymbol{M}_{\bar{\varrho}^2}$ is just five. The spectrum $\sigma_{\bar{\varrho}^2}$ consists of the spectrum σ_{ϱ^2} and of two additional eigenvalues 1. Identifying pairs of couplings with the first one, we clearly have $p_{ab} + p_{ac} = p_a$, $p_{bc} = p_b$, and $p_{ca} + p_{cc} = p_c$. Thus the vector $\boldsymbol{y}$ of the logarithms of the reduced couplings, $y_{xy} = 2\log(h_{xy}/\varepsilon_x)$, is sill perpendicular to the Perron-Frobenius eigenvector of $\boldsymbol{M}_{\bar{\varrho}}$ and converges in the renormalization limit to a linear combination of two eigenvectors $\boldsymbol{v^{1,2}}$ corresponding to an eigenvalue 1 of $\boldsymbol{M}_{\bar{\varrho}}^t$: $\boldsymbol{y} \to \log r\, \boldsymbol{v^1} + \log s\, \boldsymbol{v^2}$. While both parameters, r and s, enter the transformation matrices $\boldsymbol{M}^{\pm}$ of $\boldsymbol{\Lambda}_{\pm}$, s can actually be eliminated by a similarity transformation. Such a behaviour is always to be expected if a parameter is connected to an eigenvector (like $\boldsymbol{v^2}$ in this case) that corresponds to an *additional* eigenvalue 1 of $\boldsymbol{M}_{\bar{\varrho}^2}^t$, not contained in σ_{ϱ^2}. The Perron-Frobenius eigenvalues of $\boldsymbol{M}^{\pm}$ can be determined explicitly, and we obtain for the scaling exponent

$$z = \frac{\log\left(r + r^{-1} + 2 + \sqrt{r + r^{-1} + 3}\right)}{3\log(\tau)} \; . \tag{B.7}$$

Finally, we like to show an example of a three-letter substitution rule

$$\begin{array}{rcl} a & \to & bca \\ \varrho: \quad b & \to & bcb \\ c & \to & ca \end{array} \tag{B.8}$$

with bounded fluctuations, which nevertheless has $\lambda_2 = 1$ as the second-largest eigenvalue of the substitution matrix. This is the site substitution that corresponds to the bond-problem given by $\varrho_s : a \to aba\,;\; b \to ba$. Fluctuations are indeed bounded here, since

we just obtain the Fibonacci chain by identifying a and b, but also by identifying a and c. Calculating the scaling exponent by the above method, we obtain $z = 1$, as was to be expected.

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