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Aperiodic and correlated disorder in XY chains: exact results

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Abstract. We study thermodynamic properties, surface magnetization, specific heat and susceptibility of XY quantum chains with coupling constants following arbitrary substitution sequences. Generalizing an exact renormalization group (RG) transformation, originally formulated for Ising quantum chains, we obtain exact relevance criteria of Harris–Luck-type for this class of models. For two-letter substitution rules, a detailed classification is given of sequences leading to irrelevant, marginal or relevant aperiodic modulations. We find that the relevance of the same aperiodic sequence of couplings in general will be different for XY and Ising quantum chains. By our method, continuously varying critical exponents may be calculated exactly for arbitrary (two-letter) substitution rules with marginal aperiodicity. A number of examples are given, including the period-doubling, three-folding and precious mean chains. We also discuss extensions of the renormalization approach to a special class of long-range correlated random chains, generated by random substitutions.

1. Introduction

Phase transitions and critical phenomena in Ising spin systems with (dis-)order of various nature (random, quasiperiodic, self-similar etc) have been an active research area for many years. The main questions deal with the relevance of these kinds of disorder to the thermodynamics of different models and the characterization of new, disorder-induced universality classes. For random systems, the Harris criterion [11] gives a heuristic scaling argument for the relevance of disorder. Anticipated by work of Tracy [41] and Benza *et al* [4], this criterion has later been generalized by Luck [30] to general aperiodic disorder. Due to these arguments, the basic concept to determine the relevance of aperiodic modulations, are the *local fluctuations of the mean coupling constant* of the model. These fluctuations are measured by the so-called *wandering exponent* (or fluctuation exponent) ω. For a spin model on a regular lattice, but with varying nearest neighbour couplings $\varepsilon_{i,j}$, ω is defined as [30]

$$\sum_{\langle i,j\rangle\in V}(\varepsilon_{i,j}-\varepsilon_0)\sim|V|^{\omega}\qquad|V|\to\infty \tag{1}$$

where ε_0 is the mean coupling of the model and the sum is over all nearest neighbour pairs in a (roughly spherical) patch V with volume $|V|$. Whereas for any periodic distribution of coupling constants, fluctuations are bounded and we have $\omega = 0$, independent random couplings lead to $\omega = \frac{1}{2}$ due to the law of large numbers. The criterion now is perturbative in nature and is expected to hold for weak disorder: comparing the local shift of the critical

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point due to the aperiodic modulations with the distance from criticality, disorder should be *relevant* if the *wandering exponent* ω exceeds a critical value ω_c [30]

$$\omega_c = 1 - 1/(D\nu). \tag{2}$$

Here, ν is the correlation length exponent of the unperturbed system and the model is disordered in D coordinate directions. For the XY chain in particular, we have $D = \nu = 1$, and thus $\omega_c = 0$.

Especially since the discovery of quasicrystals in 1984, the effect of (deterministic) aperiodicity on the thermodynamical properties of different models has been the topic of numerous, mostly numerical studies. Universal behaviour was found for most quasicrystalline systems, such as Ising models on Penrose and Ammann-Beenker tilings [6, 31, 37, 39] and also in three dimensions [32]. Marginal scaling, on the other hand, has been observed for the surface roughness of two-dimensional quasicrystals [10, 12] (cf also the review [9] for further references). Although almost all results corroborate the Harris–Luck criterion, this is nevertheless somewhat more subtle for aperiodic or (more general) correlated disorder than for randomly disordered systems. This is because it is not the fluctuations of the coupling constants directly, but of the related local shift of the critical control parameter δ (the 'local reduced temperature' in classical Ising models) that should be considered. Certainly, since this quantity is rather an intuitive concept than sharply defined, its dependence on the local coupling strengths is by no means obvious in most models. While independent random couplings will normally also lead to independent local shifts of the control parameter, and therefore to fluctuations with the same fluctuation exponent $\omega = \frac{1}{2}$, this is no longer guaranteed if the coupling constants are correlated or even distributed according to a deterministic rule. The exactly solvable Ising models on the Labyrinth [3] provide an example where the strong correlations among the coupling constants due to the 'rapidity line parametrization' enforces Onsager universal behaviour even for relevant fluctuations (in the sense of [30]) of the mean coupling constant.

Analytical results have, so far, only been obtained for a small number of systems. With the exception of the Labyrinth models, which are, when solvable, somewhat non-generic in their aperiodicity, these are one-dimensional free-fermion models, such as tight-binding models or quantum chains. Most results rely, moreover, on a special choice of the aperiodic orderings (such as the Fibonacci model) which makes them applicable to efficient trace-map methods or renormalization techniques derived therefrom [1, 4, 24]. Independent of trace map properties, the surface magnetization of aperiodic *Ising quantum chains* with constant transverse field has been calculated exactly for certain substitution sequences [20]. Only recently, a decimation procedure in real space has been introduced [21] (again for particular substitution rules) that later could be generalized to obtain analytically the scaling properties of the entire class of Ising quantum chains with coupling constants following arbitrary substitution rules [13]. This led to an analytical confirmation of Luck's relevance criterion for these models.

In this paper, after a description of the model in section 2, we show in section 3 how the renormalization approach, as formulated for the Ising quantum chains, can be extended to aperiodic XY spin chains. It turns out that, for a given sequence of couplings, the influence of the induced disorder may be different in the two models. Nevertheless, fluctuations turn out to be the basic concept for the demarcation of relevant from irrelevant disorder. However, the fluctuations of the sequence of coupling constants itself and of the induced sequence of reduced coupling constants, that play the role of local critical control parameters here, behave—in contrast to the randomly disordered case—in general differently for aperiodic order. Taking this into account, the Harris–Luck relevance criterion may be adapted to XY spin chains or, equivalently, to tight-binding models with aperiodic hopping. We calculate the scaling

exponents of the surface magnetization and the central spectral gaps at criticality and derive therefrom in section 4 (following [28]) the critical scaling behaviour of the specific heat and the zero-field susceptibility. Connections to localization properties of tight-binding models are briefly mentioned. In section 5, we show how known results from trace-map approaches can be rederived, clarifying their origin in this broader context. As examples, we also give some new scaling exponents for different aperiodic chains with marginal disorder. In section 6, an extension of the renormalization approach to random substitution rules is proposed. Finally, we conclude with a short discussion.

2. The model

The system we are concerned with here is defined by the following quantum Hamiltonian:

$$H_N = -\sum_{j=1}^{N}(\varepsilon_j^x \sigma_j^x \sigma_{j+1}^x + \varepsilon_j^y \sigma_j^y \sigma_{j+1}^y). \tag{3}$$

The coupling constants $\varepsilon_j^{x,y} \geqslant 0$ are site dependent and the operators $\sigma_j^{x,y}$ denote Pauli's matrices acting on the jth site. Boundary conditions may be chosen as periodical ($\sigma_{N+1} = \sigma_1$) or free ($\varepsilon_N = 0$).

For a general set of coupling constants, this model is equivalent to a free-fermion field [27, 38], the fermionic excitation energies Λ_q satisfying the linear difference equations

$$\Lambda_q \psi_j^{(q)} = \varepsilon_{j-1}^x \phi_{j-1}^{(q)} + \varepsilon_j^y \phi_{j+1}^{(q)} \tag{4}$$

$$\Lambda_q \phi_j^{(q)} = \varepsilon_{j-1}^y \psi_{j-1}^{(q)} + \varepsilon_j^x \psi_{j+1}^{(q)}. \tag{5}$$

If we define

$$\eta_{2j}^{(q)} = \phi_{2j}^{(q)} \qquad \eta_{2j-1}^{(q)} = \psi_{2j-1}^{(q)} \tag{6}$$

$$\hat{\eta}_{2j}^{(q)} = \psi_{2j}^{(q)} \qquad \hat{\eta}_{2j-1}^{(q)} = \phi_{2j-1}^{(q)} \tag{7}$$

these equations decouple into the eigenvalue problems of two independent tight-binding models with aperiodic hopping

$$H_{tb}^{1,2} = \sum_{j=1}^{N/2}(\varepsilon_{2j}^{x,y}|2j\rangle\langle 2j+1| + \varepsilon_{2j-1}^{y,x}|2j-1\rangle\langle 2j|) + \text{h.c.} \tag{8}$$

This decoupling can also be carried out on the level of the spin chain Hamiltonian itself and has been used there to analyse XY chains with random bonds [5]. Difference operators of the kind (4), (5) underly various physical models and may also be interpreted as a phononic model with varying spring constants or the transition matrix of a one-dimensional random walk in an aperiodic environment. The Ising quantum chain with transverse magnetic field in its fermionic form also gives rise to a similar set of equations, the field variables replacing the ε^y couplings. In [13], a renormalization scheme has been defined for the case of a *uniform* magnetic field (or, more generally, field variables depending on the neighbouring coupling constants), thereby effectively decoupling the degrees of freedom that finally enter the renormalization scheme. In our situation, however, the ε^y couplings will not be determined through their neighbourhood, but, together with the ε^x couplings, follow the aperiodic sequence that defines the model.

For an equal distribution of the coupling constants over the even and odd bonds, as in the homogeneous or independent random case, the XY chain exhibits a zero temperature phase transition from an X- to a Y-ferromagnetically ordered phase at

$$\delta_\Delta := [\ln \varepsilon^x]_{\text{av}} - [\ln \varepsilon^y]_{\text{av}} = 0. \tag{9}$$

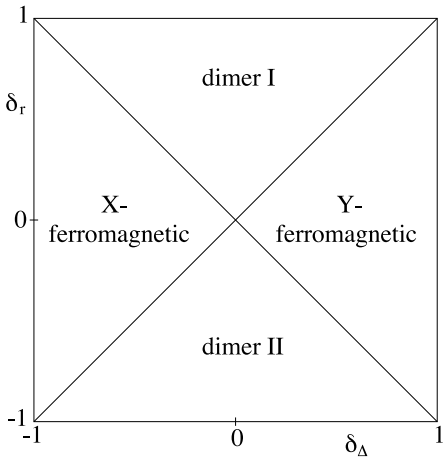

Figure 1. Phase diagram of the XY chain with ferromagnetic and dimer phases, projected to the directions δ_Δ and δ_r.

While the phase transition is of Onsager type for uniform couplings, random disorder is a relevant perturbation and leads to weaker critical singularities [38] and the peculiar properties connected to the so-called *random singlet phase* [5]. For the quasiperiodic Fibonacci sequence, a non-universal scaling law has been found for isotropic couplings ($\varepsilon_i^x = \varepsilon_i^y$) with scaling exponents depending on the coupling constants [28]. The model with *alternating* coupling constants $\varepsilon_{2j}^{x,y} = \varepsilon_e$, $\varepsilon_{2j-1}^{x,y} = \varepsilon_o$, on the other hand, shows a phase transition (again of Onsager type in the pure case) between two dimer phases [26] at

$$\delta_r := [\ln \varepsilon_{2j}^{x,y}]_{\mathrm{av}} - [\ln \varepsilon_{2j-1}^{x,y}]_{\mathrm{av}} = \ln \varepsilon_e - \ln \varepsilon_o = 0. \tag{10}$$

In the most general case the criticality condition may be obtained from the criticality conditions of the decoupled submodels (see (45) below). It compares the differences of the average (logarithmic) X and Y couplings with the difference of the average even and odd couplings of the model

$$\delta := \min\{|\delta_+|, |\delta_-|\} = 0 \qquad \delta_\pm := \delta_\Delta \pm \delta_r. \tag{11}$$

For $|\delta_\Delta| > |\delta_r|$, the model is in a ferromagnetic phase, whereas $|\delta_\Delta| < |\delta_r|$ corresponds to the dimer phases (cf figure 1).

In our models, the site-dependent coupling constants $\varepsilon_j^{x,y}$ shall be drawn from a (finite) set of values ε_{a_i}, where the label is taken from an n-letter alphabet $\mathcal{A}$ with letters $a_1, \ldots, a_n$. The aperiodic ordering of the coupling strengths in the chain is generated by an arbitrary substitution rule on the alphabet of the labels

$$\varrho : a_i \to w_i \tag{12}$$

where the w_i are *words* (finite strings of letters) from $\mathcal{A}$. As an example, consider the *silver mean* substitution rule, which reads ($a_1 = a$; $a_2 = b$):

$$\varrho_{\mathrm{sm}} : \begin{array}{lcl} a & \to & w_a = baa \\ b & \to & w_b = a \end{array} \qquad a \to baa \to abaabaa \to \ldots. \tag{13}$$

In the following, w_i^ℓ shall denote the ℓth letter and $\#_{a_j}(w_i)$ the total number of letters a_j in w_i. We also define $|w|$ to be the length (total number of letters) of a word w. Since (non-overlapping) pairs of consecutive letters will also play an important role, we finally let $\#_{\alpha\beta}(w)$ be the number of non-overlapping pairs $(\alpha\beta)$ contained in a word w of even length.

The parameters of the aperiodic model are given by the ratios of the $\varepsilon_{a_i}^{x,y}$. We define, on a logarithmic scale,

$$r_{ij} \equiv \ln \varepsilon_{a_i}^x + \ln \varepsilon_{a_i}^y - \ln \varepsilon_{a_j}^x - \ln \varepsilon_{a_j}^y \tag{14}$$

and

$$\Delta_i \equiv \ln \varepsilon_{a_i}^x - \ln \varepsilon_{a_i}^y. \tag{15}$$

The n-letter model thus contains $n-1$ independent variables which parametrize the strength of *isotropic aperiodicity* and n parameters Δ_i which determine the *aperiodic anisotropy* of the model. For notational clarity, we will restrict discussions from now on to substitution systems on a two-letter alphabet, $\mathcal{A} = \{a, b\}$, and comment only briefly on extensions to general n-letter substitutions, which can be dealt with along the same lines [15]. We also assume the following normal form for the substitution rule:

$$\varrho : \begin{array}{lcl} a & \to & w_a \equiv a w_a' \\ b & \to & w_b \equiv b w_b' \end{array} \tag{16}$$

that is, we assume the first letters of w_a and w_b to be a and b, respectively. In principle, this special form for ϱ is not needed to make our renormalization group (RG) work (see [13, 15]), but it simplifies some of the calculations. Since any two-letter substitution rule may actually be transformed into normal form without changing the model [13], our assumption does not lead to loss of generality. For the *silver mean* substitution as defined in (13) the transformation is simply done by considering the square of the original substitution rule

$$\varrho_{\mathrm{SM}} := \varrho_{\mathrm{sm}}^2 : \begin{array}{lcl} a & \to & w_a = abaabaa \\ b & \to & w_b = baa. \end{array} \tag{17}$$

The two-letter model contains three independent parameters

$$r \equiv \ln \frac{\varepsilon_a^x \varepsilon_a^y}{\varepsilon_b^x \varepsilon_b^y} \tag{18}$$

and

$$\boldsymbol{\Delta} \equiv \begin{pmatrix} \Delta_a \\ \Delta_b \end{pmatrix} = \begin{pmatrix} \ln(\varepsilon_a^x/\varepsilon_a^y) \\ \ln(\varepsilon_b^x/\varepsilon_b^y) \end{pmatrix}. \tag{19}$$

Some important statistical properties of the sequence generated by ϱ are already contained in the corresponding integer substitution matrix

$$\boldsymbol{M}_\varrho := \begin{pmatrix} \#_a(w_a) & \#_a(w_b) \\ \#_b(w_a) & \#_b(w_b) \end{pmatrix} \tag{20}$$

with eigenvalues $\lambda_\pm$. The leading eigenvalue, λ_+, gives the asymptotic scaling factor of the chain length with the number of iterated substitutions, the entries of the corresponding (statistically normalized) eigenvector, $\boldsymbol{v}_+$, determine the frequencies $p_{a,b}$ of the letters a, b in the limit chain [35]. The remaining eigenvalues of the substitution matrix are connected to fluctuation modes present in the sequence. Especially, the next-to-leading eigenvalue (here λ_-, of course) determines the wandering exponent (defined in (1) above) of the sequence of couplings [29]

$$\omega_\varepsilon = \frac{\ln|\lambda_-|}{\ln \lambda_+}. \tag{21}$$

Here, any negative value of ω_ε indicates *bounded* fluctuations in the letter frequencies, while $\omega_\varepsilon = 0$ in general is connected to *logarithmic* fluctuations [15, 29]. For the *silver mean* substitution as given by (17), we obtain

$$\boldsymbol{M}_\varrho^{\mathrm{SM}} = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix} \qquad \lambda_\pm^{\mathrm{SM}} = (1 \pm \sqrt{2})^2 \qquad \omega_\varepsilon^{\mathrm{SM}} = -1. \tag{22}$$

For the set-up of our renormalization scheme, a classification of the substitution matrices according to the fixed points of their *reductions modulo 2* will be helpful. Although this classification is mainly for technical reasons, it will become obvious that there are also differences in the physics of the models connected with the different cases. For two-letter substitution rules, there are five possible fixed points of $[M_\varrho]_{\mathrm{mod}2}$ up to the exchange of the letters a and b. They belong to three cases:

(1) Even substitutions. Here the lengths of the words w_a, w_b (the column sums of the substitution matrix) are even at the two possible fixed points:

$$(a)\quad [M_\varrho]_{\mathrm{mod}2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \left[= \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}^2 \right] \tag{23}$$

$$(b)\quad [M_\varrho]_{\mathrm{mod}2} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}. \tag{24}$$

Even substitution rules will normally lead to an unequal distribution of the letters over the even and odd positions in the sequence they generate. We thus expect the phase diagram of the corresponding XY chain to show four phases in the general case, as described above (11). The exception are substitutions where

$$p_a(\#_{ab} - \#_{ba})(w_a) + p_b(\#_{ab} - \#_{ba})(w_b) = 0 \tag{25}$$

leading to $\delta_r \equiv 0$ and a quantum chain with only two ferromagnetic phases.

(2) Odd substitutions. Here both, w_a and w_b contain an odd number of letters at the fixed points:

$$(a)\quad [M_\varrho]_{\mathrm{mod}2} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \tag{26}$$

$$(b)\quad [M_\varrho]_{\mathrm{mod}2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \left[= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^3 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}^2 \right]. \tag{27}$$

With the exception of the alternating chain with period ab, which may be generated by even and odd substitutions, the rules of this class lead to an equal distribution of all coupling constants over the even and odd bonds in the corresponding quantum chain. The phase diagram thus only contains the X- and Y-ferromagnetic phases. Our example, the *silver mean* substitution rule, belongs to this class.

(3) Mixed substitutions are neither even nor odd. For the two-letter case, we take $|w_a|$ to be odd, but $|w_b|$ to be even

$$[M_\varrho]_{\mathrm{mod}2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{28}$$

In the two-letter case, mixed substitutions behave very much like odd substitutions and lead to quantum chains without dimer phases.

Please keep in mind that any further discussion may be concentrated on the five fixed points, since any substitution rule can be transformed into an appropriate one by taking a suitable power. This clearly does not change the limit chain. In the following, we will derive relevance criteria for aperiodic disorder generated by the substitution rules of these three cases.

3. The renormalization group

In this section, we generalize the renormalization procedure introduced for the Ising quantum chain in [13]. It relies on a decimation process found in [21] for particular substitution rules and uses a special $*$-*product technique*, originally developed many years ago in the context of 1D scattering theory (see [36] and references therein).

In a first step, we now represent the *decoupled* sets of difference equations (4), (5) in terms of so-called $\mathcal{S}$ *transfer matrices*. These are defined as

$$\begin{pmatrix} \eta_{2k-1} \\ \eta_{2l} \end{pmatrix} = \mathcal{S}_{k|l} \begin{pmatrix} \eta_{2k} \\ \eta_{2l-1} \end{pmatrix} \qquad \begin{pmatrix} \hat{\eta}_{2k-1} \\ \hat{\eta}_{2l} \end{pmatrix} = \hat{\mathcal{S}}_{k|l} \begin{pmatrix} \hat{\eta}_{2k} \\ \hat{\eta}_{2l-1} \end{pmatrix}. \tag{29}$$

Since both systems are simply related under the exchange of the labels x and y, we may concentrate on the η equations from now on. Note that the η sub-model contains the ε^x-couplings of the even positions, and ε^y-couplings of the odd positions of the quantum chain.

In comparison with the ordinary transfer matrix, the $\mathcal{S}_{k|l}$ appear as scattering matrices with 'input'- and 'output'-channels exchanged. This also changes the arithmetics: the $\mathcal{S}$ matrices no longer transform by the matrix product, but by the so-called $*$-product such as

$$\mathcal{S}_{k|l} = \mathcal{S}_{k|k+1} * \mathcal{S}_{k+1|k+2} * \ldots \mathcal{S}_{l-1|l} \equiv \mathop{\Large *}_{i=1}^{l-k} \mathcal{S}_{k+i-1|k+i} \tag{30}$$

where $k < l$ and the $*$-product of two matrices is defined as

$$\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} * \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & d_2 \end{pmatrix} + \frac{1}{1 - d_1 a_2} \begin{pmatrix} b_1 c_1 a_2 & b_1 b_2 \\ c_1 c_2 & d_1 b_2 c_2 \end{pmatrix}. \tag{31}$$

The form of the elementary matrices follows from (4) and (5). For $\varepsilon^y_{2k-1} = \varepsilon^y_\alpha$, $\varepsilon^x_{2k} = \varepsilon^x_\beta$ and $\varepsilon^y_{2k+1} = \varepsilon^y_\gamma$ we obtain (dropping the eigenvalue index q)

$$\mathcal{S}_{k|k+1} \equiv \mathcal{S}_{\alpha\beta\gamma} = \begin{pmatrix} \Lambda/\varepsilon^y_\alpha & -\varepsilon^x_\beta/\varepsilon^y_\alpha \\ -\varepsilon^x_\beta/\varepsilon^y_\gamma & \Lambda/\varepsilon^y_\gamma \end{pmatrix}. \tag{32}$$

The main advantage of this form over the ordinary transfer matrix is that the fermion frequencies Λ and the ε^x-couplings are separated in the entries of (32). As we will see below, these are the two quantities to be renormalized here, while the ε^y couplings have only an indirect effect on the transformation, but keep their unrenormalized values otherwise.

The basic plan for the RG transformation is to reverse the substitution steps by $*$-multiplication of suitable blocks of $\mathcal{S}$ transfer matrices. In the corresponding problem of the aperiodic Ising quantum chain with constant transverse field $h = 1$, this is easily done. There, each $\mathcal{S}$ matrix contains only one coupling constant (ε^x_β in (32), setting all $\varepsilon^y \to h = 1$). Since every $\mathcal{S}$ matrix thus corresponds to just one letter, the renormalization steps are simply performed by $*$-multiplication of the sets of $\mathcal{S}$ transfer matrices that correspond to the words w_a or w_b in the substitution rule. With an $\mathcal{S}$ matrix depending on three consecutive coupling constants, this is no longer possible for the XY chain. In order to define the renormalization blocks for a RG transformation taking $*$-products along these blocks, we have to modify our original substitution rule ϱ. What is needed to make the renormalization procedure work, is a substitution rule on *pairs* of letters (actually rather than triples). This is because the part of a single coupling constant in the Ising chain is taken by the ratio of two consecutive coupling constants in the XY case. Note also that each ε^y coupling, according to (32), appears in two consecutive $\mathcal{S}$ matrices and the corresponding labels overlap. A substitution on n letters thus (in general) leads to a problem of dimension n^2 in the XY case—if a pair substitution rule can

be found at all†.

For the moment, let us concentrate on the cases 1 and 2 in the above classification, where a substitution rule of the desired form is easily constructed. Here, $|w_\alpha| + |w_\beta|$ is even for any $\alpha, \beta \in \{a, b\}$ and we obtain a pair substitution

$$\varrho_2 : (\alpha\beta) \to w_{\alpha\beta} \equiv w_\alpha w_\beta \tag{33}$$

with substitution matrix

$$\boldsymbol{M}_2 = \begin{pmatrix} \#_{aa}(w_{aa}) & \#_{aa}(w_{ab}) & \#_{aa}(w_{ba}) & \#_{aa}(w_{bb}) \\ \#_{ab}(w_{aa}) & \#_{ab}(w_{ab}) & \#_{ab}(w_{ba}) & \#_{ab}(w_{bb}) \\ \#_{ba}(w_{aa}) & \#_{ba}(w_{ab}) & \#_{ba}(w_{ba}) & \#_{ba}(w_{bb}) \\ \#_{bb}(w_{aa}) & \#_{bb}(w_{ab}) & \#_{bb}(w_{ba}) & \#_{bb}(w_{bb}) \end{pmatrix}. \tag{34}$$

Let $\boldsymbol{V}_i$ be the eigenvectors, and λ_i the eigenvalues of $\boldsymbol{M}_2$, λ_1 being the Perron–Frobenius one. Again, the entries $p_{\alpha\beta}$, $\alpha, \beta \in \{a, b\}$ of the corresponding eigenvector $\boldsymbol{V}_1$ determine (in statistical normalization) the frequencies of the letter pairs in the limit chain.

Since there are no pairs (bb) in the *silver mean* substitution chain, we obtain a three-dimensional pair substitution rule for this example:

$$\varrho_2^{\mathrm{SM}} : \begin{array}{ccl} (aa) & \to & (ab)(aa)(ba)(aa)(ba)(ab)(aa) \\ (ab) & \to & (ab)(aa)(ba)(ab)(aa) \\ (ba) & \to & (ba)(aa)(ba)(ab)(aa) \end{array} \qquad \boldsymbol{M}_2^{\mathrm{SM}} = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix} \tag{35}$$

with eigenvalues $\lambda_1 = (1 + \sqrt{2})^2$; $\lambda_2 = 1$; $\lambda_3 = (1 - \sqrt{2})^2$.

We now obtain a one-to-one correspondence between the letter pairs and $\mathcal{S}$ matrices if we adjoin each transfer matrix $\mathcal{S}_{\alpha\beta\gamma}$ to the pair of letters $(\alpha\beta)$ given by its first and second label.

As parameters of the RG, we now define *reduced coupling constants*

$$\mu_{\alpha\beta} \equiv \ln \varepsilon_\beta^x - \ln \varepsilon_\alpha^y \tag{36}$$

corresponding to the letter pairs. As additional parameters, we also introduce weights $\kappa_{\alpha\beta}^{\pm}$ which enter the $\mathcal{S}$ matrices in the following way:

$$\mathcal{S}_{\alpha\beta\gamma} = \begin{pmatrix} \kappa_{\alpha\beta}^{+} \Lambda / \varepsilon_\alpha^y & -\exp \mu_{\alpha\beta} \\ -(\varepsilon_\alpha^y / \varepsilon_\gamma^y) \exp \mu_{\alpha\beta} & \kappa_{\alpha\beta}^{-} \Lambda / \varepsilon_\gamma^y \end{pmatrix}. \tag{37}$$

The weight parameters account for the fact that the renormalization blocks, in general, will be asymmetric (which causes κ^+ and κ^- to differ), may contain different coupling constants and also vary in length, which results in different local weights $\kappa_{\alpha\beta}$ and $\kappa_{\alpha'\beta'}$. The arithmetic mean of the weights, however, will not be affected by RG transformation and is kept normalized

$$K^+ K^- = 1 \qquad K^{\pm} = p_{aa}\kappa_{aa}^{\pm} + p_{ab}\kappa_{ab}^{\pm} + p_{ba}\kappa_{ba}^{\pm} + p_{bb}\kappa_{bb}^{\pm} \tag{38}$$

in accordance with the initial condition $\kappa_{\alpha\beta}^{\pm} \equiv 1$.

The renormalization transformation is now obtained by reversing the substitution procedure (33)

$$\tilde{\mathcal{S}}_{\alpha\beta\gamma} \equiv \begin{pmatrix} \tilde{\kappa}_{\alpha\beta}^{+} \tilde{\Lambda} / \varepsilon_\alpha^y & \pm \exp \tilde{\mu}_{\alpha\beta} \\ \pm(\varepsilon_\alpha^y / \varepsilon_\gamma^y) \exp \tilde{\mu}_{\alpha\beta} & \tilde{\kappa}_{\alpha\beta}^{-} \tilde{\Lambda} / \varepsilon_\gamma^y \end{pmatrix} \tag{39}$$

$$\equiv \mathop{\ast}_{i=1}^{|w_{\alpha\beta}|/2} \mathcal{S}_{w_{\alpha\beta}^{2i-1} w_{\alpha\beta}^{2i} w_{\alpha\beta}^{2i+1}} \tag{40}$$

† The pair substitution needed here is entirely different from the one used to describe the Ising quantum chain with coupling constants depending on the two endpoints (site-problem), considered in [35,42]. In the Ising site problem, the chain is divided into overlapping pairs and each coupling constant appears in two pairs (with each of its neighbours), but only in one pair here. The present case may lead to a much more pronounced change in the scaling behaviour, see below.

where $w_{\alpha\beta}^{|w_{\alpha\beta}|+1} \equiv \gamma$ is the last label of the last $\mathcal{S}$ matrix in the $*$-product. It does not correspond to a letter in $w_{\alpha\beta}$, but rather to the first letter (in the first pair) of the word $w_{\alpha'\beta'}$ that defines the next renormalization block in the chain. Note that the first *letter* of every word $w_{\alpha'\beta'}$ coincides with its first *label* due to the *normal form* (16) chosen for our original substitution rule. Thus we have $\gamma = \alpha'$ here, and the labels of the renormalized $\mathcal{S}$ matrices overlap the same way as the labels of the unrenormalized matrices did, guaranteeing the consistency of the RG procedure. In our example (35), the transfer matrix connected to the pair (ab) transforms as ($\gamma \in \{a, b\}$)

$$\tilde{\mathcal{S}}_{ab\gamma} = \mathcal{S}_{aba} * \mathcal{S}_{aab} * \mathcal{S}_{baa} * \mathcal{S}_{aba} * \mathcal{S}_{aa\gamma}. \tag{41}$$

Comparing (39) and (37), we see that the ε^y-couplings just keep their values under the transformation. Their role in the RG is nevertheless non-trivial, since they affect the transformation of the weight parameters $\kappa_{\alpha\beta}$ and the ε^x-couplings (resp. the reduced couplings $\mu_{\alpha\beta}$).

Now the RG equations for the reduced couplings and weight parameters follow from the definition of the $*$-product (31). For a given substitution rule they are easily derived in explicit form in the entire parameter space, however, this will not be needed here. The transformation possesses two attractive fixed points at $\boldsymbol{\mu} = \pm\infty$, corresponding to different ordered phases of the quantum chain. The unstable critical fixed points, however, that determine the universal properties of the model will be found for a vanishing exitation gap at $\Lambda \equiv 0$. In the reminder of this section, we therefore concentrate on the RG equations of the reduced coupling constants at $\Lambda \equiv 0$, thereby analysing the fixed-point structure and the RG flow near the critical surface. The linearized RG equations of the weight parameters and fermion frequencies, on the other hand, will be needed to derive the scaling behaviour of the low-energy spectrum at criticality. This will be done in the next section.

The renormalization flow for $\Lambda \equiv 0$ follows from (31). The transformation of the reduced couplings takes a simple linear form

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{M}_2^t \boldsymbol{\mu} \tag{42}$$

where, in the two-letter case,

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_{aa} \\ \mu_{ab} \\ \mu_{ba} \\ \mu_{bb} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2\Delta_a \\ \Delta_a + \Delta_b - r \\ \Delta_a + \Delta_b + r \\ 2\Delta_b \end{pmatrix}. \tag{43}$$

The reduced coupling constants thus transform with the *transpose of the pair substitution matrix* $\boldsymbol{M}_2$. Note that the RG transformations are the same in both decoupled eigenvalue systems, however, with different initial conditions ($\Delta_{a,b} \to -\Delta_{a,b}$). The renormalization shows that the reduced couplings indeed play the role of 'local deviations from criticality': for any substitution rule, we find a fixed point of the transformation at $\boldsymbol{\mu} \equiv 0$. This is just the 'Onsager fixed-point' of the uniform model. The eigenvalues and eigenvectors of $\boldsymbol{M}_2^t$ now directly reveal the *scaling fields* u_i and *RG eigenvalues* y_i of the model

$$u_i = \boldsymbol{\mu} \cdot \boldsymbol{V}_i \qquad y_i = \frac{\ln |\lambda_i|}{\ln \lambda_1}. \tag{44}$$

In contrast to the renormalization of the Ising quantum chains, the vector of reduced couplings $\boldsymbol{\mu}$ is constrained here to a $(2n-1)$-dimensional subspace of the vector space spanned by the frequencies of n^2 different pairs of n letters. It may thus occur that certain scaling fields vanish for arbitrary choice of $\boldsymbol{\mu}$ which indicates that the corresponding fluctuational mode is not present in the problem. The contribution to the leading scaling field (with corresponding RG eigenvalue, $y_1 = 1$), however, does not vanish for a generic $\boldsymbol{\mu}$, but

$$u_1 = \boldsymbol{\mu} \cdot \boldsymbol{V}_1 = \sum_{(\alpha\beta)} p_{(\alpha\beta)} \mu_{\alpha\beta} = [\ln \varepsilon^x_{(\text{even})}]_{\text{av}} - [\ln \varepsilon^y_{(\text{odd})}]_{\text{av}} = 0 \tag{45}$$

leads to the well known criticality condition for these models (e.g. [34]). Any non-zero contribution immediately drives the sub-model off the critical surface ($\boldsymbol{\mu} \to \pm\infty$). Note, however, that the whole model is critical if the criticality condition is fulfilled for just one of the decoupled subsystems. Exchanging the labels x and y in (45) and combining the resulting expressions, we obtain the general criticality condition for the XY quantum chain, given in (11) above.

The presence of aperiodic disorder in the chain leads to non-zero contributions in the direction of the additional scaling fields. Let λ_2 be the largest eigenvalue with a non-vanishing scaling field u_2 for a generical choice of critical couplings. The corresponding RG eigenvalue y_2 is just the *wandering exponent* ω_δ of the sequence of reduced couplings, which describes the fluctuations in the local shifts of the control parameter δ

$$\omega_\delta = y_2 = \frac{\ln|\lambda_2|}{\ln\lambda_1}. \tag{46}$$

The scaling field u_2 is relevant, whenever $|\lambda_2| > 1$ and $\omega_\delta > 0$. In this case the system flows to the corresponding *strong coupling fixed point* of the RG, where the reduced couplings divide into two types, taking the values $\pm\infty$, respectively. A (simple) eigenvalue $|\lambda_2| = 1$ leads to a marginal scaling field and the system flows to a fixed line with continuously varying exponents. Finally, contributions to scaling fields with $|\lambda_2| < 1$ vanish as the RG flows to the Onsager fixed point $\boldsymbol{\mu} = 0$. Since we have $\omega_c = 0$ according to (2), this confirms the Harris–Luck criterion for these models, if the fluctuations are measured for the sequence of reduced couplings as described above. The relation of ω_δ to the fluctuation exponent ω_ε of the sequence of coupling constants itself will become clear in the following.

Before we discuss the effects of marginal or relevant aperiodicity to the critical behaviour, let us take a closer look at the spectra of the pair substitution matrices and the induced RG flows in the cases 1 and 2 above. It is worthwhile to consider for a moment the situation of *vanishing isotropic aperiodicity*. Since $r = 0$ leads to $\delta_r = 0$, the phase diagram of purely anisotropic XY quantum chains contains only the two ferromagnetic phases. Using

$$2\#_{aa}(w_{\alpha\beta}) + \#_{ab}(w_{\alpha\beta}) + \#_{ba}(w_{\alpha\beta}) = \#_a(w_\alpha) + \#_a(w_\beta) \tag{47}$$

we recognize that the vector of the anisotropy parameters $\boldsymbol{\Delta}$ transforms with the transpose of the original substitution matrix $\boldsymbol{M}_\varrho$

$$\tilde{\boldsymbol{\Delta}} = \boldsymbol{M}_\varrho^t \boldsymbol{\Delta}. \tag{48}$$

This means, however, that the fixed-point structure and the RG flow near the fixed points is identical for XY chains with aperiodic anisotropy and the aperiodic Ising spin chain analysed previously [13]. The criticality condition in this case reduces to

$$\boldsymbol{v}_+ \cdot \boldsymbol{\Delta} = 0. \tag{49}$$

Of course, (48) implies that the spectrum of $\boldsymbol{M}_\varrho$ is contained in the one of $\boldsymbol{M}_2$, and in particular $\lambda_1 = \lambda_+$. We thus have $\omega_\delta \geqslant \omega_\varepsilon$ in general, but $\omega_\delta = \omega_\varepsilon$ in the purely anisotropic case. These properties generalize literally to n letter substitutions with $|w_i|$ all even or all odd. Let us now see what happens to the RG flow when isotropic aperiodicity is turned on.

- For even substitutions, the entries of $\boldsymbol{M}_2$ are related as

$$\#_{\alpha\beta}(w_{\alpha'\beta'}) = \#_{\alpha\beta}(w_{\alpha'}) + \#_{\alpha\beta}(w_{\beta'}) \qquad \alpha, \beta, \alpha', \beta' \in \{a, b\} \tag{50}$$

  and we conclude that the spectrum of $\boldsymbol{M}_2$ is just the set $\{\lambda_+, \lambda_-, 0, 0\}$. The criticality condition derived from (45) takes the form

$$\boldsymbol{v}_+ \cdot \boldsymbol{\Delta} \pm \frac{r}{\lambda_+}[p_a(\#_{ab} - \#_{ba})(w_a) + p_b(\#_{ab} - \#_{ba})(w_b)] = 0. \tag{51}$$

With the exception of the substitutions fulfilling (25), the condition depends explicitly on r. This means that the critical manifold splits into two submanifolds for any finite strength of both, isotropic and anisotropic aperiodicity whereas the phase diagram of the isotropic chain ($\boldsymbol{\Delta} = 0$) only contains a phase transition between two dimer phases. For the exceptional cases, of course, the dimer phases are absent and the isotropic chain is always critical. In order to study the *relevance* of the aperiodic modulations, the aperiodic model should be compared with a simple homogeneous model with the same phase space topology (the model with anisotropic and alternating couplings for the general case with four phases). From the spectrum of $\boldsymbol{M}_2$ we conclude that isotropic aperiodic modulations do not lead to any further relevant or marginal scaling fields (as compared with the purely anisotropic case), but mearly renormalize the anisotropy parameters $\Delta_{a,b}$ in the first RG step. For even substitutions we thus obtain $\omega_\delta = \omega_\varepsilon$ also in the general case. The relevance of aperiodic modulations is determined by the second largest eigenvalue λ_- of the substitution matrix and is identical to the case of the Ising quantum chain. This scenario generalizes without change to the n-letter case.

- For odd substitution rules, we establish the following relations:

$$\#_{ab}(w_{aa}) = \#_{ba}(w_{aa}) \qquad \#_{ab}(w_{bb}) = \#_{ba}(w_{bb}) \tag{52}$$

$$\#_{ab}(w_{ab}) - \#_{ba}(w_{ab}) = \#_{ba}(w_{ba}) - \#_{ab}(w_{ba}). \tag{53}$$

In absence of anisotropy this means that $\boldsymbol{\mu}$ is already an eigenvector of $\boldsymbol{M}_2^t$ with eigenvalue $\lambda_{xx} = (\#_{ab} - \#_{ba})(w_{ab})$, independent of the detailed form of the substitution rule. Note that $\lambda_{xx} \leqslant \lambda_+$, and $\lambda_{xx} = \lambda_+$ only in the degenerate case where $w_{ab} = (ab)^n$ and the substitution generates the alternating chain with period ab. For all other cases, the XX chain is critical for any amount of aperiodicity induced by odd substitution rules. In the XY case, we may establish $p_{ab} = p_{ba}$ by explicit calculation of the Perron–Frobenius eigenvector of $\boldsymbol{M}_2$ and conclude that the letters a, b are indeed equally distributed over the even and odd positions in the chain. The criticality condition is thus given by (49) also in the general case and there are no dimer phases in these models. In the RG transformations, the parameters r and $\boldsymbol{\Delta}$ renormalize independently. In other words, isotropic aperiodicity leaves the anisotropy parameters unrenormalized and does not deform the critical surface, but introduces an additional scaling field in the RG. Since this may be marginal or relevant, we find $\omega_\delta = \ln|\lambda_{xx}|/\ln\lambda_+$ for the isotropic chain, but also for the general case, if $|\lambda_{xx}| > |\lambda_-|$. For the *silver mean* chain in particular, we find $\omega_\delta^{\mathrm{SM}} = 0 \neq \omega_\varepsilon^{\mathrm{SM}}$. The scaling behaviour is thus, in general, independent of the 'Ising case'. Note that the remaining eigenvalue $\lambda_4 = \delta_{w_a^{|w_a|},a} + \delta_{w_b^{|w_b|},b} - 1$ of any four-dimensional pair substitution, with eigenvector $\boldsymbol{V}_4 = (1, -1, -1, 1)^t$, does not affect the RG transformation since $\boldsymbol{\mu} \cdot \boldsymbol{V}_4 = 0$. Again, these properties generalize to n-letter substitutions with $|w_i|$ all odd. Here, isotropic aperiodicity in general leads to contributions to $n - 1$ additional scaling fields.

So far, the third case in the above classification had been set aside. Things are indeed slightly more complicated for mixed substitutions since we cannot apply our pair substitution (34) here. Nevertheless, an exact renormalization scheme may be set up also in this case. The main idea is not to construct a substitution rule for pairs of letters, but for all substrings of the chain with an even number of a and b and of minimal length (that is, they cannot be divided into smaller strings with the same property). Obviously, (aa) and (bb) are examples for such minimal strings, a general string s with length $2k \geqslant 4$ begins and ends with

a pair of letters ab or ba with an arbitrary permutation of $k-1$ pairs aa and bb in between:

$$s = \left(\left\{ \begin{matrix} ab \\ ba \end{matrix} \right\} \left\{ \begin{matrix} aa \\ bb \end{matrix} \right\}^{k-1} \left\{ \begin{matrix} ab \\ ba \end{matrix} \right\} \right). \tag{54}$$

For a given substitution rule, the number of different minimal strings is always finite, hence a substitution rule on a finite 'alphabet of different strings' s_i can always be found

$$\varrho_s : s_i \to w_{s_i} = \varrho(s_i^1)\varrho(s_i^2)\ldots \tag{55}$$

with substitution matrix

$$[\boldsymbol{M}_s]_{ij} = \#_{s_i}(w_{s_j}) \tag{56}$$

since w_{s_i} may always be dissected into minimal strings. For real space renormalization, in a first step, we contract the strings by star multiplication of the corresponding $\mathcal{S}$ transfer matrices, this way assigning a single degree of freedom to each string. After that we proceed as usual, reversing the substitution steps of the *string substitution* by decimation. Scaling fields and RG eigenvalues are again determined by the action of the transpose of the substitution matrix $\boldsymbol{M}_s$ on a scaling vector $\boldsymbol{\mu}$ with entries corresponding to the different strings, where, from the initial conditions,

$$\mu_{s_i} = \Delta_a \#_a(s_i) + \Delta_b \#_b(s_i) - r(\#_{ab} - \#_{ba})(s_i). \tag{57}$$

A more detailed analysis of the string substitution is given in the appendix, with the following results. As in the above cases, the anisotropy parameters transform with (48), leading to the Ising-like renormalization flow. For two-letter substitution rules, the effect of isotropic aperiodicity is very similar to the one described above for odd substitutions. In particular, the criticality condition (49) of the purely anisotropic case is not changed for a finite r. This means that the aperiodic XX model is always critical and dimer phases are absent in the general case. But as for odd substitutions, isotropic aperiodicity introduces a new scaling field in the model, with eigenvalue of the string substitution matrix $\lambda_s = 0$, if $(\#_{ab} - \#_{ba})(w_b) = 0$, and $\lambda_s = (2\#_{b0} - \#_b)(w_b)$ otherwise. Here, $\#_{b0}(w_b)$ gives the number of those b in w_b which leave an even number of a in the string of letters generated by cutting w_b after the letter b under consideration ($\#_a(w_1)$ even, if $w_b = w_1 b w_2$). The fluctuation exponent in the general case reads $\omega_\delta = \max\{\omega_\varepsilon, \ln|\lambda_s|/\ln\lambda_+\}$. Since $|w_b|$ is even, so is λ_s. Isotropic aperiodic modulation is thus either irrelevant or relevant, but never marginal for mixed two-letter substitutions.

Again, the question arises whether these results generalize to the n-letter case. Note that the method presented here can be applied only to a subclass of n-letter substitution rules. However, modifications are possible to treat also the most general case [15]. It turns out that the transformation of the anisotropy parameters $\Delta_{\alpha\beta}$ generalizes just as for even and odd substitutions. On the other hand, for isotropic aperiodicity, there are two possibilities. If the substitution leads to quantum chain with only the two ferromagnetic phases (as for two letters) the consequences will be as described above. But a mixed substitution may also lead to a quantum chain with dimer phases. In this case, we predict that all RG eigenvalues are given by the spectrum of $\boldsymbol{M}_\varrho$, leading to $\omega_\delta = \omega_\varepsilon$ as for even substitutions.

3.1. Critical scaling of the fermionic spectrum

The determination of the critical scaling behaviour of the lowest fermionic excitations may now be performed along the same lines as in the case of the aperiodic Ising quantum chain [13]. We will therefore only give a short account here.

We define the following vector form for the weights and fermion frequencies:

$$\boldsymbol{\Lambda}_\pm = \Lambda(\kappa_{aa}^\pm, \kappa_{ab}^\pm, \kappa_{ba}^\pm, \kappa_{bb}^\pm)^t \tag{58}$$

and consider the RG transformations of $\mathbf{\Lambda}_\pm$ to linear order in Λ. For cases 1 and 2, we obtain from (39) and (31) the linear transformation

$$\tilde{\mathbf{\Lambda}}_+ = \boldsymbol{M}^+ \mathbf{\Lambda}_+ \qquad \tilde{\mathbf{\Lambda}}_- = \boldsymbol{M}^- \mathbf{\Lambda}_- \tag{59}$$

where

$$M^+_{\alpha\beta,\alpha'\beta'} = \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w_{\alpha\beta}^{2k-1} w_{\alpha\beta}^{2k},\alpha'\beta'} \left(\frac{\varepsilon^y_\alpha}{\varepsilon^y_{w_{\alpha\beta}^{2k-1}}} \prod_{\ell=1}^{k-1} \exp(\mu_{w_{\alpha\beta}^{2\ell-1} w_{\alpha\beta}^{2\ell}}) \right)^2 \tag{60}$$

$$M^-_{\alpha\beta,\alpha'\beta'} = \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w_{\alpha\beta}^{2k-1} w_{\alpha\beta}^{2k},\alpha'\beta'} \left(\prod_{\ell=k+1}^{|w_{\alpha\beta}|/2} \exp(\mu_{w_{\alpha\beta}^{2\ell-1} w_{\alpha\beta}^{2\ell}}) \right)^2 . \tag{61}$$

At the Onsager or marginal fixed points, a similarity transformation of $\boldsymbol{M}^+$ yields the more symmetric form [13]

$$M^\pm_{\alpha\beta,\alpha'\beta'} = \exp(\mp 2\mu_{\alpha\beta}) \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w_{\alpha\beta}^{2k-1} w_{\alpha\beta}^{2k},\alpha'\beta'} \prod_{\ell=1}^{k} \exp(\pm 2\mu_{w_{\alpha\beta}^{2\ell-1} w_{\alpha\beta}^{2\ell}}). \tag{62}$$

In this form, the matrix elements are functions of the reduced couplings only. For the *silver mean* substitution (35), the matrices $\boldsymbol{M}^\pm$ read

$$\boldsymbol{M}^\pm_{\mathrm{SM}} = \begin{pmatrix} 2 + \exp(\mp r) & 1 + \exp(\mp r) & 1 + \exp(\pm r) \\ 2 & 2 & \exp(\pm r) \\ 2 & 1 & 1 + \exp(\pm r) \end{pmatrix}. \tag{63}$$

In this special case, the spectra of both transformation matrices are identical

$$\sigma(\boldsymbol{M}^\pm_{\mathrm{SM}}) = \left\{ \frac{1}{4} \left(\rho \pm \sqrt{\rho^2 + 4} \right)^2 ; 1 \right\} \qquad \rho = \exp(r/2) + \exp(-r/2). \tag{64}$$

The transformations for the string substitutions are analogous. The vectors of the weights and fermion frequencies converge under iteration of (59) to the Perron–Frobenius eigenvectors of $\boldsymbol{M}^\pm$. Using the normalization condition (38) for the weights, we now obtain the scaling behaviour of the lowest fermionic excitations. Note that the RG transformation may either by interpreted as a mapping of the low-energy spectrum of the infinite chain onto itself, or as a mapping of critical *finite-size* spectra from a system of length N to a system of length N/λ_+. Formally, we obtain the scaling of the exitation gap for a small distance from criticality

$$\Lambda \sim \delta^z \qquad \delta \to 0 \tag{65}$$

and the finite-size scaling form of the low-energy spectrum

$$\Lambda_q \sim \left(\frac{q}{N} \right)^{z'} \qquad \frac{q}{N} \ll 1 \tag{66}$$

with the scaling exponent

$$z = z' = \frac{\ln(\lambda_{M+}\lambda_{M-})}{2 \ln \lambda_+}. \tag{67}$$

Here, $\lambda_{M\pm}$ are the largest eigenvalues of $\boldsymbol{M}^\pm$.

For irrelevant aperiodic modulations, we obtain

$$\boldsymbol{M}^+ = \boldsymbol{M}^- = \boldsymbol{M}_2^t \tag{68}$$

$$\lambda_{M+} = \lambda_{M-} = \lambda_+ \tag{69}$$

and hence $z = z' = 1$. From the *finite-size scaling ansatz*, we should have $z' = z/\nu$. Thus also the Onsager value $\nu = 1$ for the correlation length exponent follows. Since the fixed-point

values of weights and couplings are independent of r and $\mathbf{\Delta}$ and thus the same as for the uniform chain we may also conclude that the low-energy excitations are equally spaced, in accordance with the predictions of *conformal invariance*. For the related problem of the Ising quantum chain, this has been observed numerically previously (e.g. [8]).

Near the marginal fixed points, the coupling constants and thus the eigenvalues $\lambda_{M\pm}$ take non-trivial values. This leads to a scaling exponent $1 < z < \infty$ which depends continuously on the coupling constants. From *finite-size scaling*, we conclude $\nu = 1$ as in the irrelevant case above. The analytic form of the scaling exponent z may be found for each substitution rule by explicit diagonalization of the four-dimensional matrices $\boldsymbol{M}^{\pm}$, see the examples below. For even substitutions, and in general for the purely anisotropic case, the RG equations may exactly be reduced to the corresponding ones of the Ising quantum chain in a transverse magnetic field. Since the scaling exponent z has been calculated there explicitly for arbitrary two-letter substitutions [13], the marginal exponent for the XY chain may also be found through this correspondence. Indeed, numerical observations indicate that not only the scaling exponents, but the entire low-energy spectra (but not the high-energy parts) of the two quantum chains are identical up to a common factor (altered fermion velocity). Note that the spectra are, of course, *not* conformally invariant for marginal fluctuations. For odd substitution rules, isotropic and anisotropic aperiodic modulation may be independently marginal. Generically, this leads to a scaling exponent depending on as many parameters as marginal scaling fields are present in the problem.

For relevant aperiodic modulations, the reduced coupling constants do not tend to a finite limit, but (generically) grow with the second largest eigenvalue λ_2 of $\boldsymbol{M}_2$. As a consequence, $\lambda_{M\pm}$ finally scales as $\lambda_{M\pm} \sim \exp(c\lambda_2^n)$ in the nth renormalization step, resulting in a scaling behaviour of the lowest gaps as

$$\Lambda_q \sim \exp(-c(N/q)^{\omega_\delta}) \tag{70}$$

with ω_δ defined in (46). Again, the same scaling behaviour, with the wandering exponent ω_ε of the sequence of couplings directly, had been found for the Ising quantum chains [29]. (See also [13] for a more detailed discussion in the Ising case.) Note that, in contrast to *random disorder*, for aperiodic sequences in general $\omega_\varepsilon \neq \omega_\delta$. The RG flow to strong couplings may lead to rather unusual critical properties, where typical and mean values of various exponents (e.g. the correlation length exponent of the spin chain) no longer coincide [5, 22], see also the discussion below. The scaling form (70) of the fermionic low-energy spectrum is, however, not affected by 'untypical events' of this type.

3.2. Critical scaling of fermionic eigenvectors

A RG transformation may also be set up for the entries of the fermionic eigenvectors, which appear in the fermionic expressions for the spin correlation functions [27]. Again, we may closely follow the analogue formulation for the Ising quantum chains, recently given in [14].

In a first step, we assign double labels to the vector entries according to the coupling pairs. This may be done in different ways, here we set $\eta_{k+1} \equiv \eta_{k+1,\alpha\beta}$ and $\eta_{k+2} \equiv \eta_{k+2,\alpha\beta}$ for $\varepsilon_k^y = \varepsilon_\alpha^y$ and $\varepsilon_{k+1}^x = \varepsilon_\beta^x$. Renormalization on the vector components acts as pure decimation; the decimated entries of the original vector are related to the renormalized ones through the $\mathcal{S}$ transfer matrices. At criticality ($\Lambda = 0$), the even and odd entries of the low-energy eigenvectors decouple and we obtain

$$C_+\eta_{2k+2i-2,w_{\alpha\beta}^{2i-1}w_{\alpha\beta}^{2i}} = \pm\frac{\varepsilon_\alpha^y}{\varepsilon^y_{w_{\alpha\beta}^{2i-1}}}\prod_{\ell=1}^{i-1}\exp(\mu_{w_{\alpha\beta}^{2\ell-1}w_{\alpha\beta}^{2\ell}})\cdot\tilde{C}_+\tilde{\eta}_{2k',\alpha\beta} \tag{71}$$

$$C_{-}\eta_{2k+2i-1,w_{\alpha\beta}^{2i-1}w_{\alpha\beta}^{2i}} = \pm \prod_{\ell=i+1}^{|w_{\alpha\beta}|/2} \exp(\mu_{w_{\alpha\beta}^{2\ell-1}w_{\alpha\beta}^{2\ell}}) \cdot \tilde{C}_{-}\tilde{\eta}_{2k'+1,\alpha\beta} \tag{72}$$

where $C_{\pm}$ are normalization factors for the even and odd components separately. In contrast to the coupling constants, the vector entries depend not only on the aperiodic label $\alpha\beta$, but also explicitly on the position k. Performing partial sums of the squared vector entries according to their aperiodic label,

$$\eta_{\alpha\beta}^{(+)} = \sum_k \eta_{2k,\alpha\beta}^2 \qquad \eta_{\alpha\beta}^{(-)} = \sum_k \eta_{2k+1,\alpha\beta}^2 \tag{73}$$

the RG transformation for the normalization factors may, however, be recast into a simple matrix form

$$C_{\pm}^2\boldsymbol{\eta}^{(\pm)} = \boldsymbol{M}^{\pm}\tilde{C}_{\pm}^2\tilde{\boldsymbol{\eta}}^{(\pm)}. \tag{74}$$

Here, $\boldsymbol{M}^{\pm}$ are in fact just the transformation matrices of the weighted fermion frequencies above (60), (61), and thus

$$C_{\pm}/\tilde{C}_{\pm} = \sqrt{\lambda_{M\pm}} \tag{75}$$

in the RG limit. The same result is obtained for the vectors $\hat{\eta}$ of the other sub-model, with $\hat{\lambda}_{M\pm}(r, \Delta) = \lambda_{M\pm}(r, -\Delta)$.

4. Thermodynamic properties

In this section the consequences of the scaling behaviour of the fermionic spectrum to the thermodynamics of the spin chain are discussed.

The X and Y surface magnetization $m_{\pm}^{x,y}$ on the left $(-)$ and right $(+)$ surfaces is the quantity expressed most easily in the fermionic representation (for simplicity we take N even). Analogous to the Ising quantum chain [23,33], it may be obtained from the large-τ limit of the imaginary time spin–spin correlation function at the surface. For free boundary conditions, this leads to an off-diagonal matrix element of the ground state with the first excited states $|1\rangle$, $|\hat{1}\rangle$ of the two decoupled submodels. These states become asymptotically degenerate with the ground state in the ordered phases [27]. Note that the ground state matrix element itself is always zero due to spin inversion symmetry. Upon expressing the boundary spins in terms of the fermions, we find the following expressions for magnetization of the left surface in the ferromagnetic phases:

$$m_{-}^{x} = \langle 1|\sigma_1^x|0\rangle = \eta_1^{(1)} \qquad m_{-}^{y} = \langle \hat{1}|\sigma_1^y|0\rangle = \hat{\eta}_1^{(1)} \tag{76}$$

and similarly for the right surface. For the marginal (or irrelevant) two-letter substitutions, we thus obtain the finite-size scaling exponent of the surface magnetization directly from the scaling of the eigenvector normalization constants considered above. For phase transitions with $\delta_r \geqslant 0$ we obtain

$$m_{\pm}^{x,y} \sim N^{-\beta_{\pm}^{x,y}/\nu} \qquad \beta_{\pm}^{x} = \frac{\ln \lambda_{M\pm}}{2\ln \lambda_{+}} \qquad \beta_{\pm}^{y} = \frac{\ln \hat{\lambda}_{M\pm}}{2\ln \lambda_{+}} \tag{77}$$

since $\nu = 1$ for irrelevant or marginal fluctuations (see above). For transitions to the dimer phase at $\delta_r < 0$, the x and y labels should formally be exchanged [15]. The surface magnetization exponents are related as

$$\beta_{+}^{x}(r, \Delta) = \beta_{-}^{x}(-r, -\Delta) = \beta_{-}^{y}(-r, \Delta) = \beta_{+}^{y}(r, -\Delta). \tag{78}$$

We also find $z = \beta_{+}^{x} + \beta_{-}^{x}$ and $\hat{z} = \beta_{+}^{y} + \beta_{-}^{y}$. In a similar way, the scaling exponent of the surface component of the so-called *string-ordering parameter* that characterizes the topological order

in the dimer phases may also be obtained [15]. In the irrelevant case, (77) gives $\beta_{\pm}^{x,y} = \frac{1}{2}$, as it should be. For marginal aperiodicity, on the other hand, the local scaling exponents of the surface magnetization do not only depend on the strength of the aperiodicity (as does z), but also explicitly on the surface of the chain: the above expressions give the exponents for a right or left surface that is itself generated by iterated substitution on an arbitrary seed (or a cut through the limit chain at a finite distance to these 'natural' surfaces). Scaling relations like (78), in general, hold only for surfaces generated that way. We give an example below for a scaling exponent β_{-}^{x} depending on the type of the surface. The gap scaling, on the other hand, is a global property and does not depend on surfaces or any other local properties of the chain.

We now proceed to the determination of the critical exponents of susceptibility and specific heat. This may be done in analogy to the analysis of the Fibonacci–XX chain in [28]. Note first that the critical scaling of the low-energy spectrum directly implies the scaling form of the integrated density of states in the thermodynamic limit as [13, 28]

$$H(\Lambda) \sim \Lambda^{1/z} g(\ln \Lambda / \ln \lambda_+) \qquad \Lambda \to 0 \tag{79}$$

(g is a function with unit period) for marginal or irrelevant aperiodicity and

$$H(\Lambda) \sim (\ln |\Lambda|)^{-1/\omega_\delta} \qquad \Lambda \to 0 \tag{80}$$

in the relevant case. The free energy (per spin) of the XY chain at finite temperature $1/\beta$ is given by an integral transform of the fermionic IDOS as [27, 28]

$$\beta f = -\frac{1}{N} \sum_q \ln(1 + \exp[\beta \Lambda_q]) \tag{81}$$

$$= -\int \mathrm{d}H(\Lambda) \ln(1 + \exp[\beta \Lambda]). \tag{82}$$

Now, the specific heat is given by

$$C_v = \beta^2 \frac{\partial^2}{\partial \beta^2}[-\beta f] = \frac{\beta^2}{4} \int \mathrm{d}H(\Lambda) \frac{\Lambda^2}{\cosh^2(\beta \Lambda/2)}. \tag{83}$$

At low temperature, this expression is dominated by the small Λ region and the $T \to 0$ scaling behaviour of C_v is completely determined through the critical scaling of the fermionic spectrum

$$C_v \sim T^{1/z} G(\ln T / \ln \lambda_+) \qquad C_v \sim 1/(\ln T)^{1+1/\omega_\delta} \tag{84}$$

for marginal (irrelevant) and relevant aperiodicity, respectively, and G is again a periodic function with unit period. Similarly, the susceptibility at vanishing field in z direction may be derived to leading order as (with $\Lambda(h) = \Lambda(h = 0) + h \cdot r(\Lambda)$, r bounded)

$$\chi_z = -\left.\frac{\partial^2 f(h)}{\partial h^2}\right|_{h=0} \sim \frac{\beta}{4} \int \frac{\mathrm{d}H(\Lambda)}{\cosh^2(\beta \Lambda/2)} \tag{85}$$

and

$$\chi_z \sim T^{1/z-1} G'(\ln T / \ln \lambda_+) \qquad \text{resp.} \quad \chi_z \sim 1/(T[\ln T]^{1/\omega_\delta}). \tag{86}$$

Thus the susceptibility diverges for any marginal or relevant aperiodic perturbation. Note that for $\omega_\delta = \frac{1}{2}$, which is the mean fluctuation exponent for uncorrelated random disorder, these expressions coincide with the scaling behaviour of the random chain [5].

As stated above, the aperiodic XY spin chain is essentially equivalent to two decoupled tight-binding models with aperiodic hopping (8). In this context, the scaling exponent z calculated above determines the *localization length* at half-filling. It is well known that the one-dimensional tight-binding model with random hopping exhibits a single delocalized state

at the band centre. This is also the case for any kind of aperiodic disorder (also due to random substitutions, see below) fulfilling the criticality condition. Using the Thouless relation [40] we obtain from (79), (80) a diverging localization length ℓ_Λ at $\Lambda = 0$, such as

$$\ell_\Lambda \sim \Lambda^{-1/z} \qquad \Lambda \to 0 \tag{87}$$

$$\ell_\Lambda \sim |\ln \Lambda|^{-1+1/\omega_\delta} \qquad \Lambda \to 0 \tag{88}$$

for marginal (or irrelevant) and relevant perturbations, respectively. A more detailed analysis of the resulting state (extended or critical) is possible for particular examples with the methods of [25].

5. Examples

- The Thue–Morse chain, generated by

$$\varrho_{TM} : \begin{matrix} a & \to & ab \\ b & \to & ba \end{matrix} \tag{89}$$

  is an even substitution of the exceptional type fulfilling (25). The model is critical whenever $\Delta_a = -\Delta_b$ and does not possess any dimer phases. The induced disorder is irrelevant, since $\lambda_- = 0$.
- The period doubling chain, generated by

$$\varrho_{pd} : \begin{matrix} a & \to & ab \\ b & \to & aa \end{matrix} \tag{90}$$

  is an example for an even substitution rule with $|\lambda_-| = 1$. The criticality condition reduces to $2\Delta_a + \Delta_b \pm r = 0$; note in particular that the *pd XX* chain is not critical. The critical scaling exponent is well known from the Ising case [21]

$$z_{pd} = \frac{\ln(2\cosh(\Delta_a/2))}{\ln 2} \tag{91}$$

  and is also for the *XY* chain a function of only one variable.
- The so-called *precious mean* (or metallic mean) chains [2,17] are generated by substitution rules with a substitution matrix of the form

$$M_k = \begin{pmatrix} k & 1 \\ 1 & 0 \end{pmatrix} \tag{92}$$

  with eigenvalues $\lambda_{k\pm} = (k \pm \sqrt{k^2+4})/2$. According to the above classification, they all belong to case 2 and are critical for $\lambda_{k+}\Delta_a = -\Delta_b$. While criticality only depends on the anisotropy parameters, the critical exponent depends solely on r. Since $|\lambda_{k-}| < 1$, anisotropic precious mean modulations are irrelevant. On the other hand, it is straightforward to check that $|\lambda_{xx}| = 1$, thus the isotropic aperiodicity is always *marginal*. For even k ($k = 2$ corresponds to the *silver mean* chain), we eliminate blocks corresponding to double substitution steps in the RG transformation and obtain the scaling exponent

$$z_k = \frac{\ln \Theta_k}{\ln \lambda_{k+}} \qquad \Theta_k = \frac{1}{4}\left(k\rho + \sqrt{k^2\rho^2 + 16}\right) \tag{93}$$

  where

$$\rho = \exp(r/2) + \exp(-r/2). \tag{94}$$

For k odd, $k = 2\ell - 1$, in each RG step three substitution steps have to be reversed. We (finally) obtain the scaling exponent

$$\tilde{z}_k = \frac{\ln \Theta_\ell}{3 \ln \lambda_{k+}} \qquad \Theta_\ell = \frac{1}{2}\left(P_\ell(r)\rho^2 + \sqrt{P_\ell^2(r)\rho^4 + 4} \right) \tag{95}$$

where

$$P_\ell(r) = \frac{\ell^2 \sinh[\ell r] + (\ell - 1)^2 \sinh[(\ell - 1)r]}{\sinh[r]} \tag{96}$$

and ρ as defined above. The first term of this series, with $k = \ell = P_1(r) \equiv 1$, corresponding to the Fibonacci chain, had already been obtained in [28] using the well known properties of the Fibonacci trace map [24]. Also for general *precious mean* chains, spectral scaling exponents may be calculated by trace maps due to the existence of invariants [2]. This has been done in [18]. Note, however, that the scaling exponents found in [18] (given in terms of Chebyshev polynomials) do not simply translate to the above expressions since the transfer matrices of the aperiodic hopping problem do not have unit determinant. In contrast to the aperiodic potential problem [18], the scaling exponents here behave differently for k even or odd in the limit of weak incommensurability $k \to \infty$. For fixed ratio of the couplings r, aperiodicity becomes irrelevant for k even ($\lim_{k\to\infty} z_k = 1$), but not for k odd ($\tilde{z}_k \to \infty$).

The *precious mean* chains are just those quasicrystalline chains that result from the so-called cut-and-project formalism with the slope of the cut space given by $\lambda_{k+} = [0, \bar{k}]$. By successive application of different precious mean substitutions, a much more general class of cut-and-project chains may be generated. Indeed, since the eigenvector $\boldsymbol{v}_{xx}$ to the marginal eigenvalue λ_{xx} of $\boldsymbol{M}_2$ is independent of k, the marginal scaling property also holds for this more general class of chains. Quadratic irrationalities in particular, which are observed in real quasicrystalline matter, are given by periodic continuous fractions and lead to cut-and-project chains that may be generated by a periodic application of precious mean substitutions. Thus the scaling exponent z can also be calculated using the above method.

Finally, we wish to stress that the origins of the marginal scaling behaviour observed for the interface roughness of Fibonacci surfaces [10, 12] and the XY quantum chains on the other hand are independent. According to the Harris–Luck criterion, the former is connected to the fact that the unperturbed correlation length exponent which enters (2) is $\nu = \frac{1}{2}$ there and the *precious mean* substitutions, being volume preserving, lead to the marginal wandering exponent $\omega_\varepsilon = -1$ [19]. Substitution rules that lead to marginal scaling in only one of these situations are easily constructed; it is rather special that the *precious mean* chains fulfil both marginality conditions.

- Different types of the three-folding chain are defined by substitution rules with substitution matrix

$$\boldsymbol{M}_{3f} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \tag{97}$$

This is one of the simplest examples of a chain where both isotropical and anisotropical aperiodicity are independently marginal (with exception of the special form $\varrho : a \to aba; b \to bab$ which leads to a periodic chain and $z = 1$). At criticality ($\Delta_a = -\Delta_b \equiv \Delta$), the continuously varying scaling exponents thus depend on two variables (ρ, Δ). Consider first two types of the substitution rule that lead to *locally isomorphic* (or patch equivalent) chains, but generate different types of surfaces:

$$\varrho_{3f_1} : \begin{matrix} a & \to & aba \\ b & \to & bba \end{matrix} \qquad \varrho_{3f_2} : \begin{matrix} a & \to & aab \\ b & \to & abb \end{matrix}. \tag{98}$$

We find the following exponents for the surface magnetization:

$$1. \quad \beta_-^x = \frac{\log[1 + \exp(r) + \exp(\Delta + r/2)]}{2\log 3} \tag{99}$$

$$2. \quad \beta_-^x = \frac{\log[1 + 2\exp(-\Delta)\cosh(r/2)]}{2\log 3}. \tag{100}$$

The gap exponent, on the other hand, is the same for all locally isomorphic chains. We obtain in any case (with ρ defined in 94)

$$z_{3f} = \frac{\ln(\rho^2 + 2\rho\cosh[\Delta] + 1)}{2\ln 3}. \tag{101}$$

The substitution rule

$$\tilde{\varrho}_{3f} : \begin{matrix} a & \to & aab \\ b & \to & bba \end{matrix} \tag{102}$$

however, generates a chain of a different local isomorphism class, and we obtain the exponents

$$\tilde{z}_{3f} = 2\beta_\pm^{x,y} = \frac{\ln \Theta_{3f}}{\ln 3} \tag{103}$$

where

$$\Theta_{3f} = \rho\cosh(\Delta) + \sqrt{[2\sinh(r/2)\sinh(\Delta)]^2 + 1}. \tag{104}$$

For $r = 0$, these expressions reduce to the corresponding ones of the Ising quantum chain [21]. Note also that $z_{3f} = \tilde{z}_{3f}$ for pure isotropic aperiodicity.

- The substitution rule

$$\varrho : \begin{matrix} a & \to & abb \\ b & \to & ababbb \end{matrix} \tag{105}$$

belongs to case 3 in the classification above. A set of four strings,

$$\{(bb), (abab), (abba), (babbba)\} \tag{106}$$

is sufficient to define a string substitution with substitution matrix

$$M_s = \begin{pmatrix} 2 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{pmatrix}. \tag{107}$$

We have $\lambda_- = 0$, hence aperiodic anisotropy is irrelevant, but since $\lambda_s = 2$ and $\omega_\delta = \ln 2/\ln 5 > 0$, isotropic aperiodicity will be relevant.

6. Extensions to correlated random disorder

Aperiodic order, as generated by substitution rules, represents a natural, but non-trivial extension of crystalline and quasicrystalline order. Structures with this type of long-range order are certainly physically reasonable (perhaps in contrast to hierarchical systems) but of course also show a number of quite special properties in comparison with random systems. These include rescaling symmetries and the *strong repetitivity* of local patches due to their self-similar structure. Moreover, the ordering is deterministic by construction and leads to zero entropy density. However, as has been argued in [29, 30], the thermodynamic properties of (quantum) spin models should be unaffected by most of these special properties, but depend only on the nature of the fluctuations present in the system. In fact, also our RG formalism

may be applied to a more general class of models and, in particular, does *not* depend on the exact self-similarity of the substitution chains. Let us explain this in more detail.

For simplicity, we concentrate on aperiodic anisotropy (respectively, the Ising case). Fix a substitution $\varrho : a_i \to w_i$, but consider the chain of couplings chosen according to the following *random substitution rule*

$$\varrho : a_i \to \mathrm{perm}(w_i) \tag{108}$$

where $\mathrm{perm}(w_i)$ denotes a random permutation of the letters in w_i. The class of chains generated this way is clearly neither deterministic nor strongly repetitive, in fact it is, almost surely, not repetitive at all. What is more, its entropy density is positive. Indeed, the nature of the fermionic spectrum is completely changed by the introduction of randomness: whereas it is typically purely *singular continuous* with a characteristic gap-structure for substitution chains, all these gaps vanish in (numerical) spectra of random substitutions. The only property that remains unchanged, is the total fluctuation of the mean (reduced) coupling. It still decomposes into a superposition of a finite number of fluctuation modes, implicitly given through the eigenvalues of the substitution matrix. This property is also the essential ingredient for our RG procedure, which depends on the substitution matrix rather than on the detailed form of the substitution itself. Consequently, neither the RG flow nor the fixed-point structure are affected by introducing randomness into the substitution rules. Note, however, that the scaling exponent z in the marginal case depends on ϱ in more detail and we only obtain analytical upper and lower bounds ($1 < z_1 \leqslant z \leqslant z_2 < \infty$) for random substitutions here [15]. Numerical results indicate that z may indeed vary within this interval and does not converge to a well defined limit.

In many respects, random substitution chains with relevant fluctuation modes (in particular, those with wandering exponent $\omega_\delta = \frac{1}{2}$) behave very similar to uncorrelated random chains. However, a characteristic difference is that for the latter only the asymptotic growth of the *mean* fluctuations is controlled by the mean deviation exponent $\omega = \frac{1}{2}$, while fluctuations of any order (up to $\omega = 1$) may be present with a non-vanishing probability on every length scale. The most significant consequence is the off-critical Griffiths phase observed in random quantum chains [5, 7], but not in aperiodic models [22]. Also, for random substitution chains with exponentially many realizations, no Griffiths phase should be present since for any non-critical values of the coupling constants there is a *finite* maximal size for 'locally critical' patches.

7. Discussion

We extended an exact real space renormalization approach, originally formulated for Ising quantum chains, to aperiodic XY quantum chains. This way, relevance criteria for aperiodic modulations have been obtained analytically for a second class of models. As predicted by the Harris–Luck relevance criterion, the geometrical fluctuation exponent plays the key role in the determination of the critical behaviour. However, the fluctuation exponent ω_δ of the sequence of ratios of consecuting ε^x and ε^y couplings, which matters for the XY models, may differ from the wandering exponent ω_ε of the sequence of interactions itself, which had been the crucial quantity in the Ising case. As a consequence, the relevance of aperiodic orderings that do not lead to a dimerization in the coupling constants ($\delta_r \equiv 0$), in general, will be different for Ising quantum chains and XY models. In particular, quasiperiodic (dis)order, generated by substitution rules compatible with the cut-and-project formalism, is irrelevant for Ising quantum chains and most other Ising spin systems, but marginal for XX or XY chains. On the other hand, aperiodic rules that lead to XY chains with dimer phases, induce fluctuations

of the same strength ($\omega_\delta = \omega_\varepsilon$) and lead to the same critical behaviour as in the Ising case.

The analysis of the RG fixed-point structure and renormalization flows in particular indicates that there is no discrimination between weak and strong aperiodic disorder in these models. The validity of the perturbative Harris–Luck criterion is thus extended to the case of strong modulations. Open questions remain mainly for relevant aperiodic disorder. Here, the RG flows to the strong coupling limit and the critical scaling behaviour of several ensemble averaged quantities is dominated by rare events. A comparison of the resulting 'aperiodic ground states' to the so-called 'random singlet phase' postulated for uncorrelated random chains [5] would be of interest. For the Ising quantum chains, a first step into that direction has been taken in [22]. We have shown that the RG approach may also be applied to random substitutions and does not rely too much on special properties of deterministic aperiodic systems. Let us remark that—especially in the Ising case—the structure of the RG is rather simple and an extension to ensembles of uncorrelated random chains should be possible. The crucial question is whether the atypical means of quantities such as the critical correlation function will be accessible within a RG scheme which works in the fermionic representation.

The renormalization approach leads to an exact determination of the scaling exponents $\beta_\pm^{x,y}$ of the surface magnetization and z of the mass gap for arbitrary two-letter substitution rules. An extension to general n-letter substitutions is possible [15]. The critical exponents connected with the scaling of the spectrum at $\Lambda = 0$ may be calculated exactly, such as the zero temperature specific heat, the susceptibility in a vanishing magnetic field in the z direction, or the localization length of the aperiodic hopping model at half-filling. We have given a number of quantitative results as examples, mainly for marginal aperiodicity.

The exact results obtained for the aperiodic XY models should be of use for the analysis (perturbational or numerical) of more complicated aperiodic models, such as XYZ spin chains. A first result for the Heisenberg chain has been obtained very recently in [16]. As for analytical results, a natural step would be to introduce a non-vanishing transverse magnetic field in z direction. However, although this still leads to a free fermion model, a treatment by exact renormalization as shown here at zero field does not seem to be a simple problem.

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Appendix. Spectra of string substitutions

We are interested in the action of the transpose string substitution matrix $\boldsymbol{M}_s^t$ on the vector $\boldsymbol{\mu}$ with

$$\mu_{s_i} = \Delta_a \#_a(s_i) + \Delta_b \#_b(s_i) - r(\#_{ab} - \#_{ba})(s_i). \tag{A.1}$$

For $\tilde{\boldsymbol{\mu}} \equiv \boldsymbol{M}_s^t \boldsymbol{\mu}$ we find

$$\tilde{\mu}_{s_i} = \Delta_a \#_a(w_{s_i}) + \Delta_b \#_b(w_{s_i}) - r(\#_{ab} - \#_{ba})(w_{s_i}). \tag{A.2}$$

Using

$$\#_a(w_{s_i}) = \#_a(w_a)\#_a(s_i) + \#_a(w_b)\#_b(s_i) \tag{A.3}$$

$$\#_b(w_{s_i}) = \#_b(w_a)\#_a(s_i) + \#_b(w_b)\#_b(s_i) \tag{A.4}$$

we obtain the transformation rule (48) of the anisotropy parameters.

On the other hand, since $|w_a|$ is odd and $|w_b|$ even, we may write

$$(\#_{ab} - \#_{ba})(w_{s_i}) = (\#_{ab} - \#_{ba})(w_b) \cdot (2\#_{b0} - \#_b)(s_i) \tag{A.5}$$

where $\#_{b0}(s_i)$ gives the number of b in $s_i = s_{i1}bs_{i2}$ with $\#_a(s_{i1})$ even. Thus isotropic aperiodicity is clearly irrelevant if $(\#_{ab} - \#_{ba})(w_b) = 0$. Otherwise, consider now the action of M_s^t on $\tilde{\boldsymbol{\mu}}$. For $\boldsymbol{\Delta} = 0$ we obtain

$$[M_s^t \tilde{\boldsymbol{\mu}}]_{s_i} = -r(\#_{ab} - \#_{ba})(w_b) \cdot (2\#_{b0} - \#_b)(w_{s_i}) \tag{A.6}$$

$$= -r(\#_{ab} - \#_{ba})(w_b) \cdot (2\#_{b0} - \#_b)(w_b) \cdot (2\#_{b0} - \#_b)(s_i) \tag{A.7}$$

and recognize $\lambda_s \equiv (2\#_{b0} - \#_b)(w_b)$ as the desired RG eigenvalue.

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