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 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 works of Tracy [39] and Benza *et. al.* [4], this criterion has later been generalized by Luck [28] to general aperiodic disorder. The argument is perturbative in nature and is expected to hold for weak disorder: Comparing the local shift of the critical point due to aperiodic modulations to the distance from criticality, disorder should be *relevant* if the so-called *wandering exponent* ω (measuring the geometrical fluctuations of the mean coupling constant) exceeds a critical value [28]

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

Here, ν is the correlation length exponent of the unperturbed system and the model is disordered in D coordinate directions.

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, 29, 37, 35] and also in three dimensions [30]. Marginal scaling, on the other hand, has been observed for the surface roughness of two-dimensional quasicrystals [12, 10]. Compare 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 in general not the fluctuations of the coupling constants directly, but of some related microscopic parameters (reduced coupling constants) that should be considered. While the statistical fluctuations of uncorrelated random couplings will normally lead to a similar fluctuational behaviour in the (a priori unknown) "reduced couplings", this is no longer guarantied if the coupling constants are correlated or even distributed according to a deterministic rule. The 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 [28]) of the mean coupling constant.

Analytical results have so far been obtained only 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 (like the Fibonacci model) which makes them applicable to efficient trace-map methods or renormalization techniques derived therefrom [23, 1, 4]. Independently of trace map properties, the surface magnetization of aperiodic *Ising quantum chains* with constant transverse field has been calculated exactly for certain substitution sequences [19]. Only recently, a decimation procedure in real space has been introduced [20] (again for particular substitution rules) that later could be generalized to obtain analytically the scaling properties of the whole 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 article, 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 determine the critical behaviour 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 [26]) 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:

$$H_N = \sum_{j=1}^{N} \left(\varepsilon_j^x \sigma_j^x \sigma_{j+1}^x + \varepsilon_j^y \sigma_j^y \sigma_{j+1}^y \right) \ . \tag{2}$$

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

For a general set of coupling constants, this model is equivalent with a free fermion field [25, 36], the fermionic excitation energies Λ_q satisfying the linear difference equations

$$\Lambda_q \psi_j^{(q)} = \varepsilon_{j-1}^x \phi_{j-1}^{(q)} + \varepsilon_j^y \phi_{j+1}^{(q)} \tag{3}$$

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

If we define

$$\eta_{2j}^{(q)} = \phi_{2j}^{(q)} \qquad \eta_{2j-1}^{(q)} = \psi_{2j-1}^{(q)} \tag{5}$$

$$\hat{\eta}_{2j}^{(q)} = \psi_{2j}^{(q)} \qquad \hat{\eta}_{2j-1}^{(q)} = \phi_{2j-1}^{(q)} \ , \tag{6}$$

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

$$H_{tb}^{1,2} = \sum_{j=1}^{N/2} \left(\varepsilon_{2j}^{x,y} |2j\rangle\langle 2j+1| + \varepsilon_{2j-1}^{y,x} |2j-1\rangle\langle 2j| \right) + h.c. \quad . \tag{7}$$

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 (3, 4) 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 uniform or randomly distributed coupling constants, the XY- chain exhibits a zero temperature phase transition from an X- to a Y-ferromagnetically ordered phase at $[\ln \varepsilon^x]_{av} = [\ln \varepsilon^y]_{av}$. 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 [26].

Here, the site-dependent coupling constants $\varepsilon_j^{x,y}$ shall be chosen according to a sequence generated by an arbitrary substitution rule

$$\varrho : a_i \ \rightarrow \ w_i \tag{8}$$

with words w_i taken from an n-letter alphabet $\mathcal{A}$ with letters $a_1, \ldots, a_n$. In the following, w_i^ℓ shall denote the ℓth letter and $\#_\alpha(w_i)$ the total number of letters α in

w_i. Since also (non-overlapping) pairs of consecutive letters will play an important role, we further define $\#_{\alpha\beta}(w)$ to give the number of pairs $(\alpha\beta)$ contained in a word w of even length. In general, let $|w|$ be the length of w.

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

$$r_{ij} \equiv \ln \varepsilon_{a_i}^{x} + \ln \varepsilon_{a_i}^{y} - \ln \varepsilon_{a_j}^{x} - \ln \varepsilon_{a_j}^{y} \tag{9}$$

and

$$\Delta_i \equiv \ln \varepsilon_{a_i}^{x} - \ln \varepsilon_{a_i}^{y} \ . \tag{10}$$

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 in most cases can be dealt with along the same lines. We assume the following normal form for the substitution rule

$$\varrho : \begin{array}{lcll} a & \to & w_a & \equiv a w'_a \\ b & \to & w_b & \equiv b w'_b \end{array} \ , \tag{11}$$

which does not impose any restriction, as any two-letter substitution rule may be transformed accordingly without changing the model [13]. In principle, the special form for ϱ is not needed to make our renormalization group work, but it simplifies some of the calculations. The two-letter model contains three independent parameters

$$r \equiv \ln \frac{\varepsilon_a^x \varepsilon_a^y}{\varepsilon_b^x \varepsilon_b^y} \tag{12}$$

and

$$\boldsymbol{\Delta} \equiv \begin{pmatrix} \Delta_a \\ \Delta_b \end{pmatrix} = \begin{pmatrix} \ln(\varepsilon_a^x / \varepsilon_a^y) \\ \ln(\varepsilon_b^x / \varepsilon_b^y) \end{pmatrix} \ . \tag{13}$$

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

$$\boldsymbol{M}_\varrho := \begin{pmatrix} \#_a(w_a) & \#_a(w_b) \\ \#_b(w_a) & \#_b(w_b) \end{pmatrix} \tag{14}$$

with eigenvalues $\lambda_\pm$. The leading eigenvalue, λ_+, gives the asymptotic scaling factor of the system size 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 word [33]. 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 fluctuation (or wandering) exponent [27]

$$\omega_\varrho = \frac{\ln |\lambda_-|}{\ln \lambda_+} \ . \tag{15}$$

For two-letter substitution rules in particular, a classification of the substitution matrices according to the fixed points of their *reductions modulo 2* will be helpful. Up to the exchange of the letters a and b, there are five possible fixed points of $[\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2}$. They belong to three cases, for which we will show the following:

1.

$$\text{a)} \qquad [\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \left[= \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}^2 \right] \tag{16}$$

$$\text{b)} \qquad [\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} \tag{17}$$

The chain is in its critical phase at $T = 0$ iff

$$\boldsymbol{v}_+ \cdot \boldsymbol{\Delta} = \pm \frac{r}{\lambda_+} \Big[p_a (\#_{ab} - \#_{ba})(w_a) + p_b (\#_{ab} - \#_{ba})(w_b) \Big] \,. \tag{18}$$

This condition holds in particular if $(\Delta_a \#_a + \Delta_b \#_b)(w_{a,b}) = \pm r (\#_{ab} - \#_{ba})(w_{a,b})$ where we find unperturbed scaling behaviour ($z = 1$). Otherwise, the relevance of the aperiodicity to the critical scaling is identical to the one for Ising quantum chains with couplings following the same aperiodic sequence: We obtain $z = 1$, marginal scaling with non-universal ($1 < z < \infty$), or random-like behaviour ($z = \infty$) for $|\lambda_-|$ smaller than, equal to, or larger than 1 respectively. Finally, off criticality, there is a gap in the fermionic integrated density of states (IDOS) at the band center.

2.

$$\text{a)} \qquad [\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \tag{19}$$

$$\text{b)} \qquad [\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \left[= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^3 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}^2 \right] \tag{20}$$

We obtain a critical ground state and a vanishing gap in the center of the IDOS iff

$$\boldsymbol{v}_+ \cdot \boldsymbol{\Delta} = 0 \,. \tag{21}$$

In particular, this implies that the model is critical for any kind of *isotropic aperiodicity* ($\Delta_a = \Delta_b = 0$). In this case, the relevance of the aperiodic modulation is determined by the renormalization group eigenvalue $\lambda_{xx} = |\#_{ab} - \#_{ba}|(w_a w_b)$ and is completely independent of the relevance of the same aperiodic ordering in the couplings of the corresponding Ising quantum chain. The relevance of *aperiodic anisotropy*, on the other hand, again agrees with the Ising case. If isotropic and anisotropic aperiodicity are both marginal, we obtain a nonuniversal scaling exponent $1 < z < \infty$ depending on two parameters.

3.

$$[\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{22}$$

The criticality condition is again given by (21). Isotropic aperiodicity is irrelevant if $\#_{ab}(w_b) = \#_{ba}(w_b)$ *or* if $2\#_{b0}(w_b) = \#_b(w_b)$. Here, $\#_{b0}(w_b)$ gives the number of b's in w_b with $w_b = w_1 b w_2$ and $\#_a(w_1)$ even. In all other cases, the induced disorder is relevant and $z = \infty$. Again, the relevance of *aperiodic anisotropy* agrees with the Ising case.

Please keep in mind that discussions 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 show how to derive these relevance criteria within an exact renormalization scheme.

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 [20] for particular substitution rules and uses a special *star-product technique*, originally developed many years ago in the context of scattering theory (see [34] and references therein).

We introduce $\mathcal{S}$ transfer matrices for the *decoupled* sets of difference equations (3, 4)

$$\begin{pmatrix} \eta_{2k-1} \\ \eta_{2l} \end{pmatrix} = \mathcal{S}_{k|l} \begin{pmatrix} \eta_{2k} \\ \eta_{2l-1} \end{pmatrix} \; ; \quad \begin{pmatrix} \hat{\eta}_{2k-1} \\ \hat{\eta}_{2l} \end{pmatrix} = \hat{\mathcal{S}}_{k|l} \begin{pmatrix} \hat{\eta}_{2k} \\ \hat{\eta}_{2l-1} \end{pmatrix} \; . \tag{23}$$

Since both systems are related under the exchange of ε^x and ε^y couplings, we may concentrate on the η equations from now on. The $\mathcal{S}$ matrices transform by $*$-products like

$$\mathcal{S}_{k|l} = \mathcal{S}_{k|k+1} * \mathcal{S}_{k+1|k+2} * \ldots \mathcal{S}_{l-1|l} \equiv \mathop{\Large *}_{i=1}^{l-k} \mathcal{S}_{k+i-1|k+i} \tag{24}$$

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

$$\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} * \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & d_2 \end{pmatrix} + \frac{1}{1-d_1 a_2} \begin{pmatrix} b_1 c_1 a_2 & b_1 b_2 \\ c_1 c_2 & d_1 b_2 c_2 \end{pmatrix} \; . \tag{25}$$

The form of the elementary matrices follows from (3, 4). 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)

$$\mathcal{S}_{k|k+1} \equiv \mathcal{S}_{\alpha\beta\gamma} = \begin{pmatrix} \Lambda/\varepsilon^y_\alpha & -\varepsilon^x_\beta/\varepsilon^y_\alpha \\ -\varepsilon^x_\beta/\varepsilon^y_\gamma & \Lambda/\varepsilon^y_\gamma \end{pmatrix} \; . \tag{26}$$

In the corresponding problem of the aperiodic Ising quantum chain with constant transverse field $h = 1$, each $\mathcal{S}$ matrix contains just one coupling constant (ε^x_β in (26), setting all $\varepsilon^y \to h = 1$), enabling an easy renormalization procedure reversing the substitution steps by $*$ multiplication of the corresponding $\mathcal{S}$ transfer matrices. With an $\mathcal{S}$ matrix depending on three consecutive coupling constants, the substitution rule has to be redefined appropriately in order to make an inverse transformation possible by taking $*$ products. As the part of a coupling constant in the Ising model is just taken by the ratio of two consecutive coupling constants in the XY case, a substitution rule on pairs of letters (actually rather than triples) is needed here to make the renormalization procedure work. The Ising problem on n letters thus corresponds to a problem of dimension n^2 in the XY case – if such a substitution rule can be found at all[1]. 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

$$\varrho_2 : (\alpha\beta) \to w_{\alpha\beta} \equiv w_\alpha w_\beta \tag{27}$$

with substitution matrix

$$\boldsymbol{M}_2 = \begin{pmatrix} \#_{aa}(w_{aa}) & \#_{aa}(w_{ab}) & \#_{aa}(w_{ba}) & \#_{aa}(w_{bb}) \\ \#_{ab}(w_{aa}) & \#_{ab}(w_{ab}) & \#_{ab}(w_{ba}) & \#_{ab}(w_{bb}) \\ \#_{ba}(w_{aa}) & \#_{ba}(w_{ab}) & \#_{ba}(w_{ba}) & \#_{ba}(w_{bb}) \\ \#_{bb}(w_{aa}) & \#_{bb}(w_{ab}) & \#_{bb}(w_{ba}) & \#_{bb}(w_{bb}) \end{pmatrix} \; . \tag{28}$$

[1] 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 end-points (site-problem), considered in [33, 40]. 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. This may lead to a much more pronounced change in the scaling behaviour, see below.

Let λ_i be the eigenvalues of $\boldsymbol{M}_2$, $\lambda_1 = \lambda_{PF}$ being the Perron-Frobenius one. We may now adjoin each transfer matrix $\mathcal{S}_{\alpha\beta\gamma}$ to the pair $(\alpha\beta)$ and define corresponding *reduced coupling constants*

$$\mu_{\alpha\beta} \equiv \ln \varepsilon^x_\beta - \ln \varepsilon^y_\alpha \ . \tag{29}$$

The renormalization transformation is now obtained by reversing the substitution procedure (27)

$$\tilde{\mathcal{S}}_{\alpha\beta\gamma} \equiv \begin{pmatrix} \tilde{\kappa}^+_{\alpha\beta}\tilde{\Lambda}/\varepsilon^y_\alpha & \pm \exp\tilde{\mu}_{\alpha\beta} \\ \pm(\varepsilon^y_\alpha/\varepsilon^y_\gamma)\exp\tilde{\mu}_{\alpha\beta} & \tilde{\kappa}^-_{\alpha\beta}\tilde{\Lambda}/\varepsilon^y_\gamma \end{pmatrix} \tag{30}$$

$$\equiv \ \mathop{\ast}_{i=1}^{|w_{\alpha\beta}|/2} \mathcal{S}_{w^{2i-1}_{\alpha\beta} w^{2i}_{\alpha\beta} w^{2i+1}_{\alpha\beta}} \tag{31}$$

where $w^{|w_{\alpha\beta}|+1}_{\alpha\beta} \equiv \gamma$. In (30), we have introduced weights $\kappa^\pm_{\alpha\beta}$ as additional parameters in our renormalization group. These 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 $\kappa_{\alpha'\beta'}$. Note that formally, in (30), only the ε^x couplings are renormalized, while the ε^y's just keep their values.

The renormalization flow on the critical surface (defined through the vanishing of the "mass gap", $\Lambda \equiv 0$) may now be directly obtained from (25) as

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{M}_2^t \boldsymbol{\mu} \tag{32}$$

where, in the 2-letter case,

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_{aa} \\ \mu_{ab} \\ \mu_{ba} \\ \mu_{bb} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2\Delta_a \\ \Delta_a + \Delta_b + r \\ \Delta_a + \Delta_b - r \\ 2\Delta_b \end{pmatrix} \ . \tag{33}$$

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 ($\Delta_{a,b} \to -\Delta_{a,b}$) of the reduced couplings. Obviously, the "Onsager fixed-point" of the uniform model just corresponds to $\boldsymbol{\mu} \equiv \boldsymbol{0}$ and the eigenvalues and eigenvectors of $\boldsymbol{M}_2^t$ directly reveal the *RG eigenvalues* and *scaling fields* of the model. The contributions in the directions of different scaling fields are measured by the scalar products of $\boldsymbol{\mu}$ with the eigenvectors $\boldsymbol{V_i}$ of $\boldsymbol{M}_2$. 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 happen 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 eigenvalue $\lambda_{PF} = \lambda_+$, see below), however, does not vanish for a generical $\boldsymbol{\mu}$, but

$$\boldsymbol{\mu} \cdot \boldsymbol{V}_{PF} = \sum_{(\alpha\beta)} p_{(\alpha\beta)} \mu_{\alpha\beta} = [\ln \varepsilon^x]_{a\,v} - [\ln \varepsilon^y]_{a\,v} = 0 \tag{34}$$

leads to the well-known *criticality condition* for these models (e.g. [32]). Any nonzero contribution immediately drives the system off the critical surface ($\boldsymbol{\mu} \to \pm\infty$) into the X or Y ferromagnetic phase. Note, however, that the whole model is critical if the criticality condition is fulfilled for just one of the decoupled subsystems.

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 for critical couplings. If this scaling field is relevant, that is, iff the *wandering exponent* of the sequence of reduced couplings is positive,

$$\omega_2 \equiv \frac{\ln|\lambda_2|}{\ln\lambda_1} > 0\,, \tag{35}$$

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 $\boldsymbol{\mu} = \mathbf{0}$. This confirms the Harris-Luck criterion for these models, since $D = \nu = 1$ for XY and Ising quantum chains, and thus $\omega_c = 0$ according to (1).

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*, $r = 0$. Using

$$2\#_{aa}(w_{\alpha\beta}) + \#_{ab}(w_{\alpha\beta}) + \#_{ba}(w_{\alpha\beta}) = \#_a(w_\alpha) + \#_a(w_\beta) \tag{36}$$

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

$$\tilde{\boldsymbol{\Delta}} = \boldsymbol{M}_\varrho^t \boldsymbol{\Delta}\,. \tag{37}$$

However, this means 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]. Of course, (37) implies that the spectrum of $\boldsymbol{M}_\varrho$ is contained in the one of $\boldsymbol{M}_2$. These properties generalize without any change 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.

- In case 1, where both $|w_a|$ and $|w_b|$ are even at the fixed point of $[\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2}$, the entries of $\boldsymbol{M}_2$ are related as

  $$\#_{\alpha\beta}(w_{\alpha'\beta'}) = \#_{\alpha\beta}(w_{\alpha'}) + \#_{\alpha\beta}(w_{\beta'})\ ;\ \alpha,\beta,\alpha',\beta' \in \{a,b\} \tag{38}$$

  and we conclude that the spectrum of $\boldsymbol{M}_2$ is just the set $\{\lambda_+, \lambda_-, 0, 0\}$. Using $\lambda_+ p_{ab} = p_a \#_{ab}(w_a) + p_b \#_{ab}(w_b)$, we recognize that the criticality condition (34) reduces to equation (18) in this case. Clearly, for substitution rules with $\#_{\alpha\beta}(w_\gamma) = \#_{\beta\alpha}(w_\gamma)\,\forall\,\alpha,\beta,\gamma$, isotropic aperiodicity is completely irrelevant. In any other case, isotropic aperiodicity and aperiodic anisotropy are coupled in (18). The critical manifold (which always has to be symmetric under the exchange of indices x and y) splits into two submanifolds corresponding to the criticality of the decoupled subsmodels (7) which intersect at $r = 0$. Put in other words, isotropic aperiodicity deforms (and splits) the critical manifold, leading to a finite renormalization of the anisotropy parameters in the first RG step, but fixed point structure and RG flows remain unchanged otherwise. The changes of the critical behaviour induced by modulated aperiodicity remain closely related to the Ising case. This scenario generalizes without change to the n-letter case.

- In case 2, $|w_a|$ and $|w_b|$ are both odd and we establish the following relations

  $$\#_{ab}(w_{aa}) = \#_{ba}(w_{aa}); \quad \#_{ab}(w_{bb}) = \#_{ba}(w_{bb}) \tag{39}$$

  $$\#_{ab}(w_{ab}) - \#_{ba}(w_{ab}) = \#_{ba}(w_{ba}) - \#_{ab}(w_{ba}) \tag{40}$$

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 $\lambda_{xx} \leq \lambda_+$, and $\lambda_{xx} = \lambda_+$ only in the degenerate case where $w_{ab} = (ab)^n$ and the limit chain is periodic (with fundamental cell ab). For all other cases, we conclude that the XX chain is critical for any amount of aperiodicity induced by substitution rules of the given form. In the XY case, the parameters r and $\boldsymbol{\Delta}$ renormalize independently. In other words, the 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, the scaling behaviour in general will be independent of the "Ising case". Note that the remaining eigenvalue $\lambda_4 = \delta_{w_a^{|w_a|},a} + \delta_{w_b^{|w_b|},b} - 1$, 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. Here, $|w_a|$ is odd and $|w_b|$ is even at the fixed point of $[\boldsymbol{M}_\varrho]_{\mathrm{mod}\,2}$. This makes things slightly more complicated since we cannot apply our pair substitution (28) here. Nevertheless, an exact renormalization scheme may be set up also in this case, at least for two-letter substitution rules. 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's and b's 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 $2k \geq 4$ begins and ends with a pair of letters ab or ba with an arbitrary permutation of $k-1$ pairs aa and bb in between:

$$s = \left(\begin{Bmatrix} ab \\ ba \end{Bmatrix} \begin{Bmatrix} aa \\ bb \end{Bmatrix}^{k-1} \begin{Bmatrix} ab \\ ba \end{Bmatrix} \right) \tag{41}$$

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

$$\varrho_s : s_i \to w_{s_i} = \varrho(s_i^1)\,\varrho(s_i^2)\ldots \tag{42}$$

with substitution matrix

$$[\boldsymbol{M}_s]_{ij} = \#_{s_i}(w_{s_j}) \tag{43}$$

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 S transfer matrices, this way assigning a single degree of freedom to each string. After that we proceed the usual way, reversing the substitution steps of the *string substitution* by decimation. Scaling fields and renormalization group 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,

$$\mu_{s_i} = \Delta_a \#_a(s_i) + \Delta_b \#_b(s_i) + r(\#_{ab} - \#_{ba})(s_i)\ . \tag{44}$$

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 (37), leading to the Ising-like renormalization flow. For two-letter substitution rules, the effect of isotropic aperiodicity is very similar to the case 2 above. A finite r does

not lead to a renormalization of the anisotropy parameters, the criticality condition is given by (21). In particular, this means that the aperiodic XX model is always critical. But as in case 2, isotropic aperiodicity introduces a new scaling field in the model, with RG eigenvalue $\lambda_s = 0$, if $(\#_{ab} - \#_{ba})(w_b) = 0$, and $\lambda_s = (2\#_{b0} - \#_b)(w_b)$ otherwise. Again, the question arises whether these results generalize to the n-letter case. Note first that the method presented here can be applied only to a subclass of n-letter substitution rules. In general, a transformation into a string substitution with strings of even length will not be possible. Within these limits (but probably also beyond) the transformation of the anisotropy parameters $\Delta_{\alpha\beta}$ generalizes just as in cases 1 and 2. On the other hand, isotropic aperiodicity in general will alter the criticality condition and renormalize $\boldsymbol{\Delta}$, but will always also introduce new scaling fields.

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. For cases 1 and 2, the RG transformations of the weights and fermion frequencies are, to linear order in Λ,

$$\tilde{\boldsymbol{\Lambda}}_+ = \boldsymbol{M}^+ \boldsymbol{\Lambda}_+ \; ; \quad \tilde{\boldsymbol{\Lambda}}_- = \boldsymbol{M}^- \boldsymbol{\Lambda}_- \tag{45}$$

where $\boldsymbol{\Lambda}_\pm = \Lambda(\kappa^\pm_{aa}, \kappa^\pm_{ab}, \kappa^\pm_{ba}, \kappa^\pm_{bb})^t$ and

$$M^+_{\alpha\beta,\alpha'\beta'} = \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w^{2k-1}_{\alpha\beta} w^{2k}_{\alpha\beta}, \alpha'\beta'} \left(\frac{\varepsilon^y_\alpha}{\varepsilon^y_{w^{2k-1}_{\alpha\beta}}} \prod_{\ell=1}^{k-1} \exp(\mu_{w^{2\ell-1}_{\alpha\beta} w^{2\ell}_{\alpha\beta}}) \right)^2 \tag{46}$$

$$M^-_{\alpha\beta,\alpha'\beta'} = \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w^{2k-1}_{\alpha\beta} w^{2k}_{\alpha\beta}, \alpha'\beta'} \left(\prod_{\ell=k+1}^{|w_{\alpha\beta}|/2} \exp(\mu_{w^{2\ell-1}_{\alpha\beta} w^{2\ell}_{\alpha\beta}}) \right)^2 . \tag{47}$$

For the derivation of (46), the special form of the substitution rule (11) is used. At the Onsager or marginal fixed points, a similarity transformation of $\boldsymbol{M}^+$ yields the more symmetric form [13]

$$M^\pm_{\alpha\beta,\alpha'\beta'} = \exp(\mp 2\mu_{\alpha\beta}) \sum_{k=1}^{|w_{\alpha\beta}|/2} \delta_{w^{2k-1}_{\alpha\beta} w^{2k}_{\alpha\beta}, \alpha'\beta'} \prod_{\ell=1}^{k} \exp(\pm 2\mu_{w^{2\ell-1}_{\alpha\beta} w^{2\ell}_{\alpha\beta}}) \tag{48}$$

In this form, the matrix elements are functions of the reduced couplings alone. The transformations in case 3 are analogous. The vectors of the weights and fermion frequencies converge under iteration of (45) to the Perron-Frobenius eigenvectors of $\boldsymbol{M}^\pm$ and the scaling behaviour of the lowest fermionic excitations ($q \ll N$) is then given by the normalization condition of $\boldsymbol{\Lambda}_\pm$ as [13]

$$\Lambda_q \sim \left(\frac{q}{N}\right)^z \; ; \quad z = \frac{\ln(\lambda_{M+}\lambda_{M-})}{2\ln\lambda_+} \tag{49}$$

where $\lambda_{M\pm}$ are the largest eigenvalues of $\boldsymbol{M}^\pm$. For irrelevant aperiodic modulations, we obtain

$$\boldsymbol{M}^+ = \boldsymbol{M}^- = \boldsymbol{M}_2^t \tag{50}$$

$$\lambda_{M+} = \lambda_{M-} = \lambda_+ \tag{51}$$

and hence $z = 1$. 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 before (e.g. [8]).

Near the marginal fixed points, the coupling constants and thus the eigenvalues $\lambda_{M\pm}$ take non-trivial values. For aperiodic anisotropy ($r = 0$), the RG equations may exactly be reduced to the corresponding ones of the Ising quantum chain in a constant transverse magnetic field ($h = 1$), with coupling constants $\varepsilon^2_{a,b} = \exp(\Delta_{a,b})$. Indeed, numerical observations indicate that not only the scaling exponents, but the entire low energy spectra are identical up to a common factor (altered fermion velocity). Note that this correspondence does of course not extend to the entire (high energy) spectrum. The scaling exponent z has been calculated explicitly for arbitrary two-letter substitutions in [13]. After a proper renormalization of $\mathbf{\Delta}$, also the exponents of marginal substitutions of case 1 are found easily through this correspondence. For substitution rules of the second case, isotropic and anisotropic aperiodic modulation may be independently marginal. Generically, this leads to a scaling exponent $1 < z < \infty$ depending on as many parameters as marginal scaling fields are present in the problem. Especially in the n-letter case, however, there are also exceptional substitutions, where marginal RG eigenvalues are in fact *marginally irrelevant*, leading to $z = 1$, or also lead to a *marginally relevant* scaling behaviour with $z = \infty$, see [15] for a discussion.

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 like $\lambda_{M\pm} \sim \exp(c\lambda_2^n)$ in the nth renormalization step, resulting in a scaling behaviour of the lowest gaps as (see [13] for a more detailed discussion in the Ising case)

$$\Lambda_q \sim \exp(-c(N/q)^{\omega_2}) \tag{52}$$

with ω_2 defined in (35). Again, the same scaling behaviour, with the wandering exponent ω_ϱ of the sequence of couplings directly, had been found for the Ising quantum chains [27]. Note that, contrary to *random disorder*, for aperiodic sequences in general $\omega_\varrho \neq \omega_2$.

In general, 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 critical exponent of the spin chain) no longer coincide [5, 21], see also the discussion below. The scaling exponent z to be calculated here 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 [25]. Again, we may closely follow the analog 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 $\varepsilon^y_k = \varepsilon^y_\alpha$ and $\varepsilon^x_{k+1} = \varepsilon^x_\beta$. 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

$$C_+\eta_{2k+2i-2,w_{\alpha\beta}^{2i-1}w_{\alpha\beta}^{2i}} = \pm\frac{\varepsilon_\alpha^y}{\varepsilon_{w_{\alpha\beta}^{2i-1}}^y}\prod_{\ell=1}^{i-1}\exp(\mu_{w_{\alpha\beta}^{2\ell-1}w_{\alpha\beta}^{2\ell}})\cdot\tilde{C}_+\tilde{\eta}_{2k',\alpha\beta} \tag{53}$$

$$C_-\eta_{2k+2i-1,w_{\alpha\beta}^{2i-1}w_{\alpha\beta}^{2i}} = \pm\prod_{\ell=i+1}^{|w_{\alpha\beta}|/2}\exp(\mu_{w_{\alpha\beta}^{2\ell-1}w_{\alpha\beta}^{2\ell}})\cdot\tilde{C}_-\tilde{\eta}_{2k'+1,\alpha\beta} \tag{54}$$

where $C_\pm$ are normalization factors for the even and odd components separately. Contrary 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,

$$\eta_{\alpha\beta}^{(+)} = \sum_k \eta_{2k,\alpha\beta}^2 \; ; \quad \eta_{\alpha\beta}^{(-)} = \sum_k \eta_{2k+1,\alpha\beta}^2 \; , \tag{55}$$

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

$$C_\pm^2\,\boldsymbol{\eta}^{(\pm)} = \boldsymbol{M}^\pm\tilde{C}_\pm^2\,\tilde{\boldsymbol{\eta}}^{(\pm)} \; . \tag{56}$$

Here, $\boldsymbol{M}^\pm$ are in fact just the transformation matrices of the weighted fermion frequencies above (46,47), and thus

$$C_\pm/\tilde{C}_\pm = \sqrt{\lambda_{M\pm}} \tag{57}$$

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

4 Thermodynamical 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 to be expressed most easily in the fermionic representation (for simplicity we take N even). Analogous to the Ising quantum chain [31, 22], 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 a 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 [25]. 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 for the left surface

$$m_+^x = \langle 1|\sigma_1^x|0\rangle = \eta_1^{(1)} \; ; \quad m_+^y = \langle\hat{1}|\sigma_1^y|0\rangle = \hat{\eta}_1^{(1)} \; . \tag{58}$$

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

$$m_\pm^{x,y} \sim N^{-\beta_\pm^{x,y}/\nu} \; ; \quad \beta_\pm^x/\nu = \frac{\ln\lambda_{M\pm}}{2\ln\lambda_+} \; , \; \beta_\pm^y/\nu = \frac{\ln\hat{\lambda}_{M\pm}}{2\ln\lambda_+} \; . \tag{59}$$

Since correlations are not dominated by "atypical events" for bounded or marginal fluctuations, the correlation length critical exponent keeps its unperturbed value

$\nu = 1$ (this may also be shown with methods of [22]), and the surface magnetization exponents are related as $\beta_+^x(r,\Delta) = \beta_-^x(-r,-\Delta) = \beta_-^y(-r,\Delta) = \beta_+^y(r,-\Delta)$. We also find $z = \beta_+^x + \beta_-^x$ and $\hat{z} = \beta_+^y + \beta_-^y$. Keep in mind, however, that the critical surfaces of the two submodels in general do not coincide.

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 [26]. Note first that the critical scaling of the low-energy spectrum directly implies the scaling form of the integrated density of states in the thermodynamical limit as [26, 13]

$$H(\Lambda) \sim \Lambda^{1/z} g(\ln\Lambda/\ln\lambda_+)\,; \quad \Lambda \to 0 \tag{60}$$

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

$$H(\Lambda) \sim (\ln|\Lambda|)^{-1/\omega_2}\,; \quad \Lambda \to 0 \tag{61}$$

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 [25, 26]

$$\beta f = -\frac{1}{N}\sum_q \ln\left(1+\exp[\beta\Lambda_q]\right) \tag{62}$$

$$= -\int \mathrm{d}H(\Lambda)\ln(1+\exp[\beta\Lambda])\,. \tag{63}$$

Now, the specific heat is given by

$$C_v = \beta^2\frac{\partial^2}{\partial\beta^2}\left[-\beta f\right] = \frac{\beta^2}{4}\int \mathrm{d}H(\Lambda)\frac{\Lambda^2}{\cosh^2(\beta\Lambda/2)}\,. \tag{64}$$

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

$$C_v \sim T^{1/z} G(\ln T/\ln\lambda_+)\,; \quad C_v \sim 1/(\ln T)^{1+1/\omega_2} \tag{65}$$

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)

$$\chi_z = -\left.\frac{\partial^2 f(h)}{\partial h^2}\right|_{h=0} \sim \frac{\beta}{4}\int \frac{\mathrm{d}H(\Lambda)}{\cosh^2(\beta\Lambda/2)}\,. \tag{66}$$

and

$$\chi_z \sim T^{1/z-1} G'(\ln T/\ln\lambda_+) \quad \text{resp.} \quad \chi_z \sim 1/(T[\ln T]^{1/\omega_2}) \tag{67}$$

Thus the susceptibility diverges for any marginal or relevant aperiodic perturbation. Note that for $\omega_2 = 1/2$, 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 (7). 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 center. 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 [38] we obtain from (60,61) a diverging localization length ℓ_Λ at $\Lambda = 0$, like

$$\ell_\Lambda \sim \Lambda^{-1/z} \; ; \qquad \Lambda \to 0 \tag{68}$$

$$\ell_\Lambda \sim |\ln \Lambda|^{-1+1/\omega_2} \; ; \quad \Lambda \to 0 \tag{69}$$

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 [24].

5 Examples

- The Thue-Morse chain, generated by

$$\varrho_{TM} : \left\{ \begin{array}{lcl} a & \to & ab \\ b & \to & ba \end{array} \right. \tag{70}$$

  belongs to case 1 and is critical whenever $\Delta_a = -\Delta_b$. The induced disorder is irrelevant, since $\#_{ab}(w_{ab}) = \#_{ba}(w_{ab})$.

- The period doubling chain, generated by

$$\varrho_{pd} : \left\{ \begin{array}{lcl} a & \to & ab \\ b & \to & aa \end{array} \right. \tag{71}$$

  is an example of a substitution rule of case 1 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 [20]

$$z_{pd} = \frac{\ln(2\cosh(\Delta_a/2))}{\ln 2} \tag{72}$$

  and is also for the XY- chain a function of only one variable.

- The so-called precious mean (or metallic mean) chains [16, 2] are generated by substitution rules with a substitution matrix of the form

$$\boldsymbol{M}_k = \begin{pmatrix} k & 1 \\ 1 & 0 \end{pmatrix} \tag{73}$$

  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

$$z_k = \frac{\ln \Theta_k}{\ln \lambda_{k+}} \; , \quad \Theta_k = \frac{1}{4}\left(k\rho + \sqrt{k^2\rho^2 + 16}\right) \tag{74}$$

  where

$$\rho = \exp(r/2) + \exp(-r/2) \; . \tag{75}$$

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

$$\tilde{z}_k = \frac{\ln \Theta_\ell}{3 \ln \lambda_{k+}} , \quad \Theta_\ell = \frac{1}{2} \left(P_\ell(r) \rho^2 + \sqrt{P_\ell^2(r) \rho^4 + 4} \right) , \tag{76}$$

where

$$P_\ell(r) = \frac{\ell^2 \sinh[\ell r] + (\ell - 1)^2 \sinh[(\ell - 1) r]}{\sinh[r]} \tag{77}$$

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 [26] using the well-known properties of the Fibonacci trace map [23]. Also for general precious mean chains, spectral scaling exponents may be calculated by trace maps due to the existence of invariants. This has been done in [17]. Note however that the scaling exponents found in [17] (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 [17], 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 which 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 holds also 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 also the scaling exponent z can be calculated using the above method.

Finally, we like to stress that the origins of the marginal scaling behaviour observed for the interface roughness of Fibonacci surfaces [12, 10] 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 (1) is $\nu = 1/2$ there and the precious mean substitutions, being volume preserving, lead to the marginal wandering exponent $\omega_\varrho = -1$ [18]. 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 fulfill both marginality conditions.

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

$$\boldsymbol{M}_{3f} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{78}$$

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). We obtain (for both submodels)

$$z_{3f} = \frac{\ln(\rho^2 + 2\rho \cosh[\Delta] + 1)}{2 \ln 3} \quad \text{for} \quad \varrho_{3f} : \begin{array}{ccc} a & \to & aab \\ b & \to & bab \end{array} \tag{79}$$

and substitution rules that lead to *locally isomorphic* (or patch equivalent) chains, and

$$\tilde{z}_{3f} = \frac{\ln \Theta_{3f}}{\ln 3} \quad \text{for} \quad \tilde{\varrho}_{3f} : \begin{array}{lcl} a & \to & aab \\ b & \to & bba \end{array} \tag{80}$$

where $\Theta_{3f} = \rho \cosh(\Delta) + \sqrt{[2\sinh(r/2)\sinh(\Delta)]^2 + 1}$. For $r = 0$, these expressions reduce to the corresponding ones of the Ising quantum chain [20]. Note also that $z_{3f} = \tilde{z}_{3f}$ for pure isotropic aperiodicity.

- The substitution rule

$$\varrho : \left\{ \begin{array}{lcl} a & \to & abb \\ b & \to & ababbb \end{array} \right. \tag{81}$$

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

$$\{(bb), (abab), (abba), (babbba)\}\,, \tag{82}$$

is sufficient to define a string substitution with substitution matrix

$$\boldsymbol{M}_s = \begin{pmatrix} 2 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{pmatrix} . \tag{83}$$

We have $\lambda_- = 0$, hence aperiodic anisotropy is irrelevant, but since $\lambda_s = 2$ and $\omega_2 = \ln 2 / \ln 5 > 0$, isotropic aperiodicity will be relevant.

6 Extensions to correlated random disorder

Aperiodic order, as generated by substitution rules, represents a natural, but nontrivial 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 to 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 [27, 28], the thermodynamical 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*

$$\varrho : a_i \to \mathrm{perm}(w_i) \tag{84}$$

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 ($1 < z_1 \leq z \leq z_2 < \infty$) 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 $\omega_2 = 1/2$) 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 $\omega = 1/2$, 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 [7, 5], but not in aperiodic models [21]. 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_2 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_ϱ of the sequence of interactions itself, which had been the crucial quantity in the Ising case. As a consequence, the relevance of the same aperiodic ordering of the coupling constants in general will be different for Ising quantum chains and isotropic XX models. In particular, quasi-periodic (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 XY anisotropy leads to identical fluctuations and 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 done in [21]. 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 like 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 $\beta^{x,y}/\nu$ of the surface magnetization and z of the mass gap for arbitrary two-letter substitution rules and quite general classes of n-letter substitutions. The critical exponents connected with the scaling of the spectrum at $\Lambda = 0$ may be calculated exactly, like the zero temperature specific heat, the susceptibility in a vanishing magnetic field in 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 (analytical and numerical) of more complicated aperiodic models, like Heisenberg and XYZ spin chains. 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 A: 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 (37) 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's in $s_i = s_{i1} b s_{i2}$ with $\#_a(s_{i1})$ even. Thus isotropic aperiodicity is clearly irrelevant if $(\#_{ab} - \#_{ba})(w_b) = 0$. Otherwise, consider now the action of $\boldsymbol{M}_s^t$ on $\tilde{\boldsymbol{\mu}}$. For $\boldsymbol{\Delta} = 0$ we obtain

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

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

and recognize $\lambda_s \equiv (2\#_{b0} - \#_b)(w_b)$ as the desired RG eigenvalue. Since $|w_b|$ is even, so is λ_s, isotropic aperiodic modulation is thus either irrelevant or relevant, but never marginal in this case.

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