Nonperiodic Ising Quantum Chains and Conformal Invariance

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In a recent paper, Luck investigated the critical behavior of one-dimensional Ising quantum chains with coupling constants modulated according to general nonperiodic sequences. In this note, we take a closer look at the case where the sequences are obtained from (two-letter) substitution rules and at the consequences of Luck's results at criticality. They imply that only for a certain class of substitution rules is the long-distance behavior still described by the $c = 1/2$ conformal field theory of a free Majorana fermion as for the periodic Ising quantum chain, whereas the general case does not lead to a conformally invariant scaling limit.

1. INTRODUCTION

In this note, we consider the Ising quantum chain with ferromagnetic exchange couplings $\varepsilon_j > 0$ which follow an, in general, nonperiodic sequence of finitely many different values. For convenience, we choose the (constant) transversal field to be equal to one, and consider the Hamiltonians

$$H^{(\pm)} = -\tfrac{1}{2}\left(\sum_{j=1}^{N} \varepsilon_j \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^{N} \sigma_j^z \right) \tag{1.1}$$

of (anti-) periodic approximants ($\sigma_{N+1}^x = \pm \sigma_1^x$) obtained by truncating the sequence of exchange couplings to the first N elements. Here, σ_j^x denotes

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the Pauli matrix σ^x acting on site j of an N-fold tensor product space. Note that $H^{(\pm)}$ commutes with the operator

$$Q = \prod_{j=1}^{N} \sigma_j^z, \qquad Q^2 = Id \tag{1.2}$$

which has eigenvalues ± 1. We denote the projectors onto the corresponding eigenspaces (sometimes also called sectors) by

$$P_{\pm} = \tfrac{1}{2}(Id \pm Q) \tag{1.3}$$

In ref. 1, the Hamiltonian (1.1) is formulated in terms of fermionic operators by means of a Jordan–Wigner transformation[2] and diagonalized by a suitable Bogoljubov–Valatin transformation. To be more precise, it is in fact the so-called mixed sector Hamiltonian[3] $\tilde{H}^{(+)}$ defined by

$$\tilde{H}^{(\pm)} = H^{(\pm)}P_+ + H^{(\mp)}P_- \tag{1.4}$$

which is considered. This is necessary since the Jordan–Wigner transformation of $H^{(\pm)}$ produces nonlocal boundary terms in the fermionic operators, whereas the above Hamiltonians (1.4) corresponds to periodic (resp. antiperiodic) boundary conditions in terms of the fermions.

Let us cite three results of ref. 1 which are central to our subsequent discussion. The system described by the Hamiltonian (1.1), resp. (1.4), is critical at $\mu = 0$ with

$$\mu = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \log(\varepsilon_j) \tag{1.5}$$

The dispersion relation for the low-energy one-particle excitations with energy Λ takes the form

$$\Lambda^2 = v^2(q^2 + \mu^2) \tag{1.6}$$

where q denotes the momentum, and v, the velocity of elementary excitations, is given by

$$\frac{1}{v^2} = \lim_{N \to \infty} \frac{1}{N^2} \sum_{j=1}^{N} \sum_{k=1}^{N} \prod_{l=1}^{k} \varepsilon_{j+l-1}^2 \tag{1.7}$$

provided the latter limit exists.

In what follows, we consider sequences of coupling constants which are obtained by substitution rules, focusing on the case of two-letter substitution rules (although most properties can be generalized quite easily to the n-letter case).

2. SUBSTITUTION RULES AND MATRICES

We consider two-letter substitution rules

$$\rho: \quad \begin{cases} a \to w_a \\ b \to w_b \end{cases} \tag{2.1}$$

where w_a and w_b are words in a and b (we do not allow for inverses of a or b here). If one defines multiplication of words through concatenation, the action of ρ is extended to arbitrary words in a and b via the homomorphism property $\rho(w_a w_b) = \rho(w_a)\,\rho(w_b)$; for details see ref. 4 and references included therein. To ρ we associate a 2×2 matrix $\mathbf{R}_\rho$

$$\mathbf{R}_\rho = \begin{pmatrix} \#_a(w_a) & \#_a(w_b) \\ \#_b(w_a) & \#_b(w_b) \end{pmatrix} \tag{2.2}$$

whose elements count the number of a's and b's in the words w_a and w_b, respectively. Note that we use the transpose matrix in comparison with ref. 4 because we need only the *statistical* eigenvectors in our discussion. They are then the right-eigenvectors of $\mathbf{R}_\rho$. With this convention, one also has $\mathbf{R}_{\rho \circ \sigma} = \mathbf{R}_\rho \cdot \mathbf{R}_\sigma$. By using the substitution rule ρ of (2.1) iteratively on an initial word $w(0)$, say $w(0) = a$ for definiteness, one obtains a sequence of words $w(n) = \rho(w(n-1))$. Since we are interested in sequences which have a unique limit word w, we restrict ourselves to substitution rules where w_a begins with the letter a. In this case, the sequence $w(n) = \rho(w(n-1))$ obviously commences with $w(n-1)$ and thus each iteration only appends letters to the previous word. The length (i.e., the number of letters) of the word $w(n)$ is given by $f_\rho(n)$ defined as follows:

$$e_\rho(n) = \begin{pmatrix} e_\rho^{(a)}(n) \\ e_\rho^{(b)}(n) \end{pmatrix} = \mathbf{R}_\rho e_\rho(n-1), \qquad e_\rho(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$f_\rho(n) = e_\rho^{(a)}(n) + e_\rho^{(b)}(n) \tag{2.3}$$

We denote the eigenvalues of $\mathbf{R}_\rho$ in (2.2) by $\lambda_\rho^{(\pm)}$, where $\lambda_\rho^{(+)}$ stands for the Perron–Frobenius eigenvalue. The corresponding statistically normalized eigenvector is determined by

$$\mathbf{R}_\rho \begin{pmatrix} p_a \\ p_b \end{pmatrix} = \lambda_\rho^{(+)} \begin{pmatrix} p_a \\ p_b \end{pmatrix}, \qquad p_a + p_b = 1 \tag{2.4}$$

The eigenvalue $\lambda_\rho^{(+)}$ determines the asymptotic inflation factor for one substitution, whereas p_a (p_b) is the frequency of the letter a (resp. b) in the limit word. Let us now discuss under which conditions $\lambda^{(-)}$ contains some information about fluctuations.

3. FLUCTUATIONS

Consider the truncated sequences $w^{(N)}$ of the first N letters of the limit word w obtained from the substitution rule (2.1) with initial word a. To measure the fluctuation, we define

$$g(N) = \#_a(w^{(N)}) - p_a N, \qquad g_n = g(f_\rho(n)) \qquad (3.1)$$

and

$$h(N) = \max_{M \leqslant N} |g(M)|, \qquad h_n = h(f_\rho(n)) \qquad (3.2)$$

Note that it does not matter whether we look at fluctuations in the frequency of the letter a or b, since $\#_a(w^{(N)}) + \#_b(w^{(N)}) = N$ and $p_a + p_b = 1$. Hence, $g(N)$ just changes sign if one replaces a by b in Eqs. (3.1) and (3.2). Of course, if $\lambda_\rho^{(+)}$ is not degenerate, $\lim_{N \to \infty}(g(N)/N) = 0$.

The behavior of $g(N)$ for words of length $N = f_\rho(n)$ which correspond to proper (or complete) iteration steps is governed by the second largest eigenvalue $\lambda^{(-)}$.[1] In fact, writing the starting vector $e_\rho(0)$ of (2.3) as a linear combination of the eigenvectors of $\mathbf{R}_\rho$ of (2.2), one easily verifies $g_n \sim \lambda^{(-)n}$. Hence $|\lambda^{(-)}| < 1$ implies that g_n converges to zero for $n \to \infty$. On the other hand, if $|\lambda^{(-)}| > 1$, then g_n in general diverges. In the limiting case of $|\lambda^{(-)}| = 1$, $|g_n|$ is constant and therefore is bounded away from zero *and* infinity. This observation brings along, once again, the concept of Pisot–Vijayaraghavan (PV) numbers.[5] They are real algebraic integers $\vartheta > 1$ all algebraic conjugates of which (except ϑ) lie inside the unit circle. If the characteristic polynomial of $\mathbf{R}_\rho$ is irreducible over the integers and if the Perron–Frobenius eigenvalue is larger than 1, the PV property really is what determines the conformal nature of the critical point. The same seems still to be true if the characteristic polynomial is reducible but all eigenvalues except the largest one lie inside the unit circle—in which case we say that the underlying substitution has bounded fluctuation property. However, the reducible case requires some care, as we will demonstrate by an example.

To understand why this is so important, one has to realize that these considerations only apply to words which are obtained by proper iteration steps. In between, fluctuations can behave quite differently, especially in the so-called marginal case $|\lambda^{(-)}| = 1$.[1,6] There, depending on the actual substitution rule (and not on the substitution matrix alone), one can have the situation that $h(N)$ is bounded or that $h(N)$ diverges logarithmically with N (or, in other words, h_n diverges linearly with n). If $|\lambda^{(-)}| > 1$, $h(N)$ can diverge like a power law. Again, polynomials reducible over the integers are to be treated carefully, in particular for generalizations to the n-letter case.

As an illustrative example, consider the substitution rules that have the substitution matrix

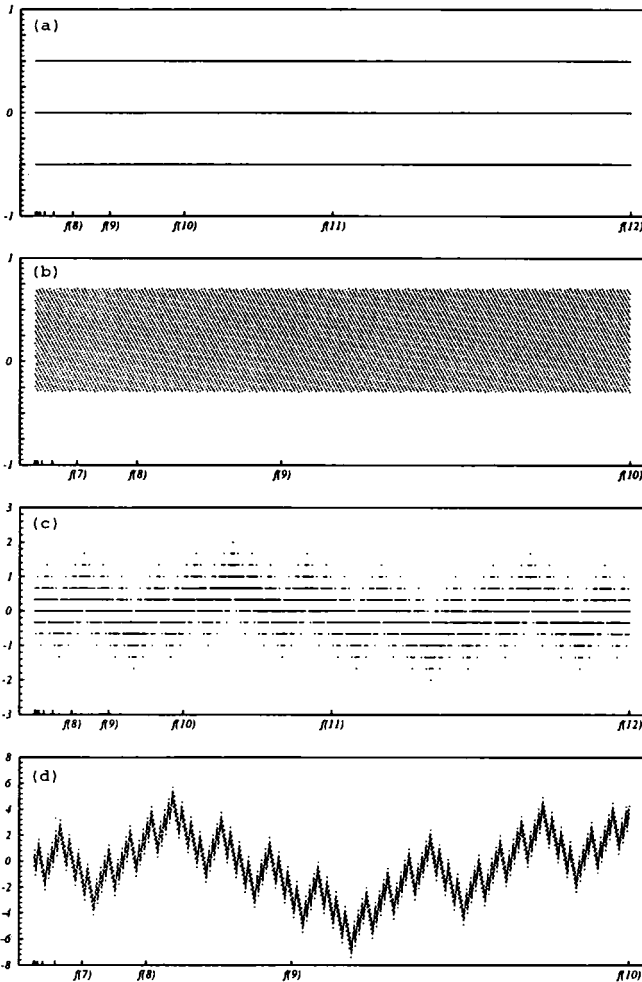$$\mathbf{R}_\rho = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{3.3}$$

Fig. 1. Fluctuations $g(N)$ [see (3.1)] for the following sequences: (a) Thue–Morse, (b) silver mean, (c) period-doubling, and (d) binary non-Pisot. The lengths of sequences which correspond to complete iteration steps are indicated.

with eigenvalues $\lambda^{(+)} = 3$ and $\lambda^{(-)} = 1$, and $p_a = p_b = 1/2$. To obtain a unique limit word, we want w_a to commence with a, which leaves us with six different substitution rules:

$$\rho_1: \begin{cases} a \to aab \\ b \to abb \end{cases} \quad \rho_2: \begin{cases} a \to aab \\ b \to bab \end{cases} \quad \rho_3: \begin{cases} a \to aab \\ b \to bba \end{cases} \tag{3.4}$$

$$\rho_4: \begin{cases} a \to aba \\ b \to abb \end{cases} \quad \rho_5: \begin{cases} a \to aba \\ b \to bab \end{cases} \quad \rho_6: \begin{cases} a \to aba \\ b \to bba \end{cases}$$

Of these, ρ_5 is special in the sense that it leads to the periodic sequence *abababab*..., which means that in this case the fluctuations are certainly bounded (since in any finite part the numbers of a's and b's differ at most
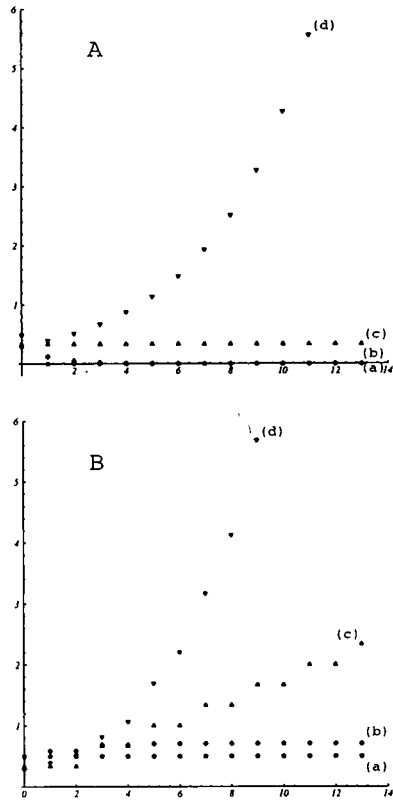

Fig. 2. (A) Fluctuations $|g_n|$, (3.1), and (B) h_n, (3.2), for the following sequences: (a) Thue–Morse, (b) silver mean, (c) period-doubling, and (d) binary non-Pisot.

by one). As it turns out, this is only true for this special sequence, in all the five other cases h_n grows linearly with n. More precisely, one observes

$$2h_n = \begin{cases} n+1 & \text{for } \rho_1, \rho_2, \text{ and } \rho_3 \\ n & \text{for } \rho_4 \\ 1 & \text{for } \rho_5 \\ \max(1, n-1) & \text{for } \rho_6 \end{cases} \tag{3.5}$$

for $n \geqslant 0$.

In Fig. 1, we show the different behavior of the fluctuations $g(N)$ for four typical substitution rules, (a) the Thue–Morse sequence, (b) the silver mean sequence (sometimes also called "octonacci" sequence), (c) the period-doubling sequence, and (d) the binary non-Pisot sequence. The substitution rules which define these sequences together with their statistical properties are summarized in Table I. Figure 2 shows the quantities $|g_n|$ of (3.1) and h_n of (3.2) for the different sequences. The marginal case of the period-doubling sequence ($\lambda^{(-)} = -1$) clearly shows the linear divergence of h_n in n, whereas $|g_n|$ is constant.

4. CRITICAL POINT AND FERMION VELOCITY

We now come back to the Hamiltonian (1.4). We relate the coupling constants ε_j to a substitution rule ρ, (2.1), in the following way:

$$\varepsilon_j = \begin{cases} \varepsilon_a & \text{if } j\text{th letter in } w \text{ is } a \\ \varepsilon_b & \text{if } j\text{th letter in } w \text{ is } b \end{cases} \tag{4.1}$$

The condition $\mu = 0$, (1.5) for criticality now reads

$$p_a \log(\varepsilon_a) + p_b \log(\varepsilon_b) = 0 \tag{4.2}$$

which has the one-parameter solution[7,8]

$$\varepsilon_a = r^{-p_b}, \qquad \varepsilon_b = r^{p_a} \tag{4.3}$$

where $r > 0$ is any positive real number.

As is well known (see ref. 9 and references therein), the finite-size scaling limit of the periodic Ising quantum chain (which corresponds to $r = 1$) is described by the $c = 1/2$ conformal field theory of a free Majorana fermion. To obtain a conformally invariant scaling limit one has to have a linear dispersion relation at criticality, which means that the limit in Eq. (1.7) must exist. This in turn is only to be expected if the fluctuations

Table I. Four Typical Substitution Rules and the Statistical Properties of the Corresponding Sequences

Sequence	Substitution rule	Eigenvalues $\lambda^{(\pm)}$	Values of p_a and p_b	p_a/p_b
Thue–Morse	$\rho_{tm}: \begin{cases} a \to ab \\ b \to ba \end{cases}$	$2, 0$	$1/2, 1/2$	1
Silver mean	$\rho_{sm}: \begin{cases} a \to aab \\ b \to a \end{cases}$	$1 \pm \sqrt{2}$	$1 - \sqrt{2}/2, \sqrt{2}/2$	$\sqrt{2} - 1$
Period-doubling	$\rho_{pd}: \begin{cases} a \to ab \\ b \to aa \end{cases}$	$2, -1$	$2/3, 1/3$	2
Binary non-Pisot	$\rho_{bnp}: \begin{cases} a \to ab \\ b \to aaa \end{cases}$	$(1 \pm \sqrt{13})/2$	$(5 - \sqrt{13})/2, (-3 + \sqrt{13})/2$	$(1 + \sqrt{13})/2$

$g(N)$ remain bounded, i.e., $h_n < S(\rho)$ for all n, since at criticality one obtains from Eqs. (3.1) and (4.3)

$$\prod_{j=1}^{N} \varepsilon_j = r^{-g(N)} \tag{4.4}$$

and all products of this type enter in Eq. (1.7). On the other hand, if the limit in Eq. (1.7) does exist, the scaling limit will be the same as for the periodic quantum Ising chain.

Although we are not going to use it in this note, we should add that there is a very elegant and efficient way to investigate this kind of system by means of the corresponding trace map (see refs. 4 and 8 and references therein). In this context, the critical point is obtained from a unique one-parameter family of bounded orbits in the accessible phase space region of the trace map.[8]

5. FERMION AND CONFORMAL SPECTRUM

We now consider the spectrum of the Hamiltonian (1.4) at criticality. It is described in terms of N fermion frequencies $\Lambda_k \geqslant 0$. In Fig. 3, we present the integrated density of the Λ_k (which we divided by their largest value for convenience) for coupling constants defined by $r = 2$ [see (4.3)] and several sizes of the chain. In general there are no exact degeneracies in the spectrum, in contrast to the periodic case. However, as the size of the system increases, the frequencies tend to accumulate, which creates the nearly vertical steps in Fig. 3, especially close to the maximal frequency. The plots show characteristic gaps in the fermion spectrum the locations of which (on the vertical axis) are in accordance with the general gap labeling theorem.[10,11,4] We should mention, though, that the Thue–Morse chain does not show closed gaps here, in contrast to the situation with electronic spectra of Schrödinger operators,[12] a phenomenon that deserves further exploration.

For models whose continuum limit is described by a conformal field theory, conformal invariance specifies the behavior of the ·low-energy excitations in the infinite-size limit $N \to \infty$. Essentially, they have to show a leading $1/N$ behavior and the level and degeneracy structure of the spectrum (after appropriate overall scaling of the gaps) are described by representations of the Virasoro algebra with central extension c, which is the central charge of the conformal field theory (see, e.g., refs. 9, 13, and 14). This of course means that it is the *lower part* of the integrated fermion density shown in Fig. 3 which is important for the conformal spectra.

To have a closer look at this part, we consider the scaled energy gaps

$$\bar{E}_j = \frac{N}{2\pi v} (E_j - E_0) \tag{5.1}$$

of the Hamiltonian $\tilde{H}^{(+)}$ of (1.4), where E_0 denotes the ground-state energy and v is the velocity of elementary excitations. For the Thue–Morse
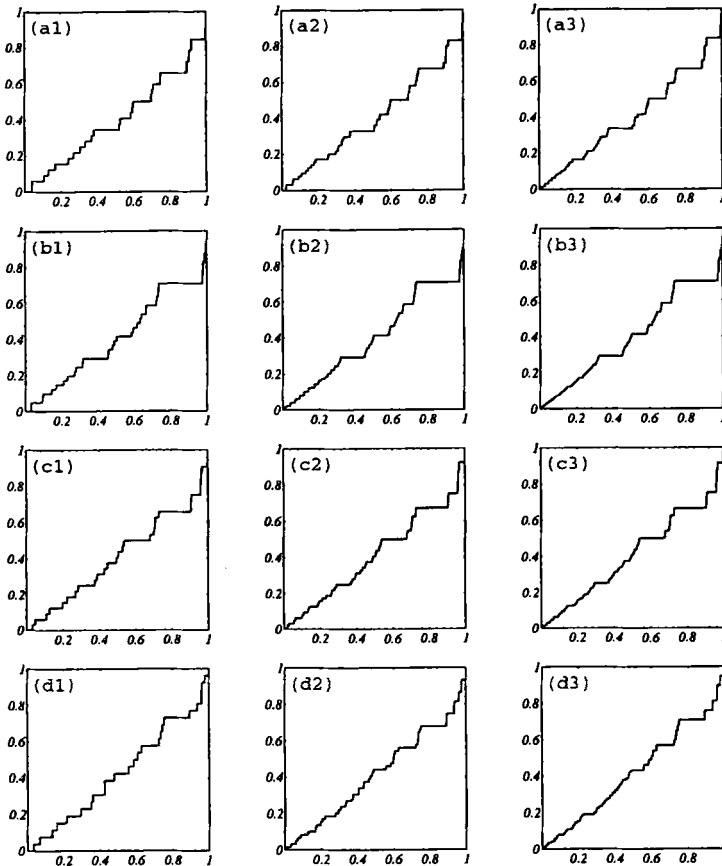

Fig. 3. Integrated density of normalized fermion frequencies for the Hamiltonian $\tilde{H}^{(+)}$ of (1.4). The coupling constants are given by Eq. (4.3) with $r = 2$ and: (a1)–(a3) the Thue–Morse sequence with $n = 5$, 6, 7, (b1)–(b3) the silver mean sequence with $n = 4$, 5, 6, (c1)–(c3) the period-doubling sequence with $n = 5$, 6, 7, and (d1)–(d3) the binary Non-Pisot sequence with $n = 4$, 5, 6, where n denotes the number of iterations. The spectra do not have true degeneracies, and the integrated density reaches 1 in all cases shown.

and the silver mean sequences, v is finite (in the limit $N \to \infty$ and for finite $r > 0$) and given by[1]

$$v = \begin{cases} \left(\dfrac{r^{1/2} + r^{-1/2}}{2} \right)^{-2} & \text{for the Thue–Morse chain} \\ \left(\dfrac{r - r^{-1}}{2} \right)^{-1} \log(r) & \text{for the silver mean chain} \end{cases} \tag{5.2}$$
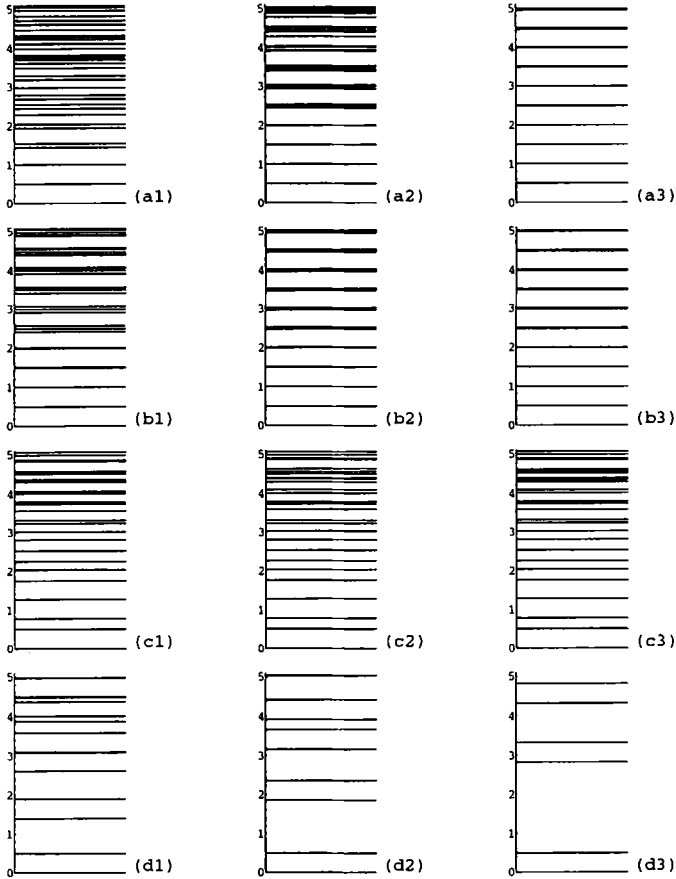

Fig. 4. Scaled low-energy spectra of $\tilde{H}^{(+)}$, (1.4), for couplings obtained from Eq. (4.3) with $r = 2$ and: (a1)–(a3) the Thue–Morse sequence with $n = 6$, 7, 8, (b1)–(b3) the silver mean sequence with $n = 5$, 6, 7, (c1)–(c3) the period-doubling sequence with $n = 6, 7, 8$, and (d1)–(d3) the binary non-Pisot sequence with $n = 5$, 6, 7, where n denotes the number of iterations. Normalization of (a) and (b) is taken from (5.2), while for (c) and (d) the first gap is normalized to $1/2$.

In fact, the second value generally applies for all quasiperiodic sequences[1] which can be obtained from a certain section through a higher-dimensional periodic structure via the dualization method.[15] On the other hand, the symmetric random dimer chain yields the same result as the Thue–Morse chain.[1] It thus represents a disordered model (with bounded fluctuations) which nevertheless shows the same critical behavior as the periodic Ising chain and, in particular, leads to a conformally invariant continuum limit.

From our discussion of the fluctuations and from Eq. (1.7) above it is clear that for the period-doubling and binary non-Pisot sequences the fermion velocity v should vanish. In Fig. 4, the scaled spectrum of low-energy excitations is shown for our four exemplary sequences. For the Thue–Morse and silver mean chains, the fermion velocity (5.2) is used, whereas for the other two sequences we simply normalize the first gap to 1/2. (We did not systematically investigate the scaling laws here, although this might give independent access to the critical exponents calculated in ref. 1.) The formation of the so-called conformal towers can be seen clearly for the spectra of the Thue–Morse and silver mean chains (a look at the actual data confirms that the degeneracies are those predicted from conformal invariance), whereas the spectra of the other two systems do not show any apparent regularities. As expected, the normalization factors grow with the size of the system in these cases. As a consequence, the nature of the critical point is quite different,[1] and conformal invariance is lost.

6. CONCLUDING REMARKS

The interest in conformally invariant phase transitions and the almost immediate study of quasiperiodic systems of the Fibonacci type (see, e.g., refs. 7 and 16–18) originally led to the somewhat misleading conclusion that conformal invariance is robust with respect to many sorts of order or even disorder. Although this is true for quasiperiodic Ising quantum chains (because that implies the PV property or the bounded fluctuation property[19]), many other ordered structures can be defined which destroy conformal invariance at the critical point. Even more, one can consider the bounded fluctuation situation to be somewhat exceptional (e.g., PV numbers are nowhere dense in $[1, \infty)$[20] and thus conclude that the general case of a nonperiodic Ising quantum chain does not lead to a conformally invariant scaling limit.

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REFERENCES

1. J.-M. Luck, Critical behavior of the aperiodic quantum Ising chain in a transverse magnetic field, *J. Stat. Phys.* **72**:417 (1993).
2. E. Lieb, T. Schultz, and D. Mattis, Two soluble models of an antiferromagnetic chain, *Ann. Phys.* (N.Y.) **16**:407 (1961); reprinted in: *Mathematical Physics in One Dimension*, E. H. Lieb and D. C. Mattis, eds. (Academic Press, New York, 1966).
3. M. Baake, P. Chaselon, and M. Schlottmann, The Ising quantum chain with defects (II), *Nucl. Phys. B* **314**:625 (1989).
4. M. Baake, U. Grimm, and D. Joseph, Trace maps, invariants, and some of their applications, *Int. J. Mod. Phys. B* **7**:1527 (1993).
5. J. W. S. Cassels, *An Introduction to Diophantine Approximation* (Cambridge University Press, Cambridge, 1957).
6. J. M. Dumont, Summation formulae for substitutions on a finite alphabet, in: *Number Theory and Physics*, J.-M. Luck, P. Moussa, and M. Waldschmidt, eds. (Springer, Berlin, 1990).
7. V. G. Benza, Quantum Ising quasi-crystal, *Europhys. Lett.* **8**:321 (1989).
8. J. A. G. Roberts and M. Baake, Trace maps as 3D reversible dynamical systems with an invariant, Melbourne preprint 9-1992; *J. Stat. Phys.*, to appear.
9. J. L. Cardy, Conformal invariance, in: *Phase Transitions and Critical Phenomena*, vol. 11, C. Domb and J. L. Lebowitz, eds. (Academic Press, New York, 1987).
10. J. Bellissard, K-theory of C^*-algebras in solid state physics, in: *Statistical Mechanics and Field Theory: Mathematical aspects*, T. C. Dorlas, N. M. Hugenholtz, and M. Winnik, eds. (Springer, Berlin, 1986).
11. J. Bellissard, A. Bovier, and J. M. Ghez, Gap labelling theorems for one-dimensional discrete Schrödinger operators, *Rev. Math. Phys.* **4**:1 (1992).
12. J. Bellissard, Spectral properties of Schrödinger's operator with a Thue–Morse potential, in: *Number Theory and Physics*, J.-M. Luck, P. Moussa, and M. Waldschmidt, eds. (Springer, Berlin, 1990).
13. J. L. Cardy, Conformal invariance and statistical mechanics, in: *Fields, Strings and Critical Phenomena, Les Houches, Session 49, 1988*, E. Brézin and J. Zinn-Justin, eds. (North-Holland, Amsterdam, 1990).
14. P. Ginsparg, Applied conformal field theory, in: *Fields, Strings and Critical Phenomena, Les Houches, Session 49, 1988*, E. Brézin and J. Zinn-Justin, eds. (North-Holland, Amsterdam, 1990).
15. P. Kramer and M. Schlottmann, Dualisation of Voronoi domains and Klotz construction: A general method for the generation of proper space fillings, *J. Phys. A* **22**:L1097 (1989).
16. H. A. Ceccatto, Phase transition in aperiodic spin chains, *Z. Phys. B* **75**:253 (1989).
17. J. Q. You, X. Zeng, T. Xie, and J. R. Yan, Quantum Heisenberg–Ising models on generalized Fibonacci lattices, *Phys. Rev. B* **44**:713 (1991).
18. M. Henkel and A. Patkós, On the restoration of translational invariance in the critical quantum Ising model on a Fibonacci chain, *J. Phys. A* **25**:5223 (1992).
19. E. Bombieri and J. E. Taylor, Which distributions of matter diffract? An initial investigation, *J. Phys.* (Paris) **C3**:19 (1986).
20. D. W. Boyd, The distribution of the Pisot numbers in the real line, in: *Séminaire de Théorie des Nombres*, C. Goldstein, ed. (Birkhäuser, Boston, 1985).