

Random and aperiodic quantum spin chains: A comparative study

F. Iglói^{1,2,a}, D. Karevski², and H. Rieger^{3,b}

¹ Research Institute for Solid State Physics, 1525 Budapest, P.O.Box 49, Hungary

² Laboratoire de Physique des Matériaux, Université Henri Poincaré, 54506 Vandœuvre-les-Nancy, France

³ HLRZ, Forschungszentrum Jülich, 52425 Jülich, Germany

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Abstract. According to the Harris-Luck criterion the relevance of a fluctuating interaction at the critical point is connected to the value of the fluctuation exponent ω . Here we consider different types of relevant fluctuations in the quantum Ising chain and investigate the universality class of random as well as deterministic-aperiodic models. At the critical point the random and aperiodic systems behave similarly, due to the same type of extreme broad distribution of the energy scales at low energies. The critical exponents of some averaged quantities are found to be a universal function of ω , but some others do depend on other parameters of the distribution of the couplings. In the off-critical region there is an important difference between the two systems: there are no Griffiths singularities in aperiodic models.

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The presence of quenched disorder has a profound effect on quantum phase transitions, especially in one dimension [1]. A common feature of these one-dimensional random magnets is the extremely broad distribution of energy scales at low energies in the vicinity of the critical point. This property makes it possible to use approximate renormalization-group transformations [2], which becomes exact at the critical point. Recently, Fisher [3] has obtained new striking results for the random transverse-field Ising spin chain defined by the Hamiltonian:

$$H = - \sum_l J_l \sigma_l^x \sigma_{l+1}^x - \sum_l h_l \sigma_l^z. \quad (1)$$

Here the σ_l^x , σ_l^z are Pauli matrices at site l and the J_l exchange couplings and the h_l transverse-fields are random variables. The random couplings (and fields) in (1) show unbounded fluctuations, the cumulated deviation from the average coupling $[J]_{\text{av}} = \int dJ J P(J)$, where $P(J)$ is the probability distributions of the couplings, grows asymptotically with the size L as:

$$\Delta(L) = \sum_{l=1}^L (J_l - [J]_{\text{av}}) \sim L^\omega, \quad (2)$$

with the fluctuating or wandering exponent $\omega = \omega_{\text{rand}} = 1/2$. A similar type of unbounded fluctuations occur in

aperiodic sequences, too, which are generated through substitutional rules. For example the Rudin-Shapiro (RS) sequence is built on four letters A, B, C and D with the substitutional rule:

$$A \rightarrow AB, \quad B \rightarrow AC, \quad C \rightarrow DB, \quad D \rightarrow DC, \quad (3)$$

thus starting with a letter A one proceeds as: $A \rightarrow AB \rightarrow ABAC \rightarrow ABACABDB \rightarrow \text{etc.}$, and one may assign different couplings to the different letters. The wandering exponent of the sequence

$$\omega = \ln |A_2| / \ln A_1, \quad (4)$$

which is given in terms of the leading and the next-to-leading eigenvalues $A_{1,2}$ of the substitution matrix [4], is $\omega_{\text{RS}} = 1/2$, *i.e.* just the same as for the random sequence.

Then naturally the question arises, which type of critical behavior can be found in quantum Ising chains with an unbounded aperiodic modulation in the couplings (or fields). It is known from the Harris-Luck relevance-irrelevance criterion [5,6] that the phase transition in an aperiodic (or quasi-periodic) quantum Ising chain belongs to the universality of the *classical* Ising model in two dimensions, only if the fluctuations in the couplings are bounded, $\omega < 0$. For marginal sequences with $\omega = 0$ non-universal critical behavior and coupling dependent anisotropy exponent was found in exact calculations [7–9].

In the relevant situation with $\omega > 0$ there are only a few exact results [10], however, on the basis of scaling considerations [6,9–11] the phase transition in relevantly aperiodic and random systems seem to be similar.

^a Permanent address also: Institute for Theoretical Physics, Szeged University, 6720 Szeged, Hungary

^b e-mail: heiko@hlrz.kfa-juelich.de

For instance the energy gap of a finite, aperiodic chain at the critical point scales as:

$$\Delta E(L) \sim \exp(-\text{const.} \times L^\omega), \quad (5)$$

just as in the random model [3, 12, 13]. Thus one could ask the question, whether the wandering exponent ω alone is sufficient to characterize the universality classes of models with fluctuating interactions; and whether or not the critical exponents of the random and the RS chains are the same?

To answer these questions here we are going to study systematically the critical behavior of aperiodic quantum spin chains with unbounded fluctuations and compare it with that of the random system. We mainly concentrate on the RS model, but some results are also presented for a family of relevant sequences defined on k -letters (k -general sequence) A_1, A_2, \dots, A_k , with the substitutional rules $A_i \rightarrow A_{i-1}A_{i+1}$ for $i \leq k/2$ and $A_i \rightarrow A_{i+1}A_{i-1}$ for $i > k/2$ (one identifies $A_0 = A_1$ and $A_{k+1} = A_k$). The wandering exponent (4) for the k -general sequences, given by

$$\omega_k = \ln[2 \cos(\pi/k)] / \ln 2, \quad (6)$$

is positive for $k \geq 4$. It is easy to see that the k -general sequence for $k = 2$ and $k = 4$ is just the Thue-Morse and the Rudin-Shapiro sequence, respectively, and obviously $\omega_4 = \omega_{\text{RS}} = 1/2$.

In the Hamiltonian (1) we have chosen homogeneous fields $h_l = h$ and two-valued couplings: $J_l = \lambda$ for letters A_i with $i < (k+1)/2$, and $J_l = 1/\lambda$ for letters with $i > (k+1)/2$. For an odd k we take $J_l = 1$ for $i = (k+1)/2$. Similarly, for the random model we take homogeneous fields and binary distribution of the couplings: $J_l = \lambda$ and $J_l = 1/\lambda$, with the same probability. The critical point, simply given by [3, 14]:

$$[\ln J]_{\text{av}} = [\ln h]_{\text{av}}, \quad (7)$$

is at $h_0 = 1$, both for the random and aperiodic systems.

In the following we calculate different physical quantities (energy-gap, surface and bulk magnetization, critical magnetization profiles, correlation length, *etc.*) for the RS-chain and compare with the known results on the random chain. We also present some results for the k -general chains, more details will be given in a subsequent publication [15]. In the actual calculation, we first transform H in equation (1) into a fermionic model [16] and then use the representation in reference [7], which necessitates only the diagonalization of a $2L \times 2L$ tridiagonal matrix. The energy gap then corresponds to the smallest positive eigenvalue of the matrix, whereas the magnetization profiles can be obtained from the corresponding eigenvectors. Details will be presented elsewhere [15].

We are going to calculate the *average* quantities of finite systems both for the random and aperiodic chains. For the aperiodic systems the average is performed as follows. We consider an infinite sequence through substitutions, cut out sequels of length L , which start at all different points of the sequence and then average over the

realizations. Among these realizations there are $R(L)$ different, which grows linearly with L : $R(L) = aL$. For the RS-chain the number of different realizations is less than $16L$, and one can obtain the *exact* average value by the following procedure. Consider the RS-sequence in (3) generated from a letter A, take the first $4L$ sequels of length L , starting at positions $1, 2, \dots, 4L$ and take also their reflexion symmetric counterparts. Then repeat the procedure starting with a letter D. The averaging then should be performed over these $16L$ realizations. The fact that the number of different samples grows linearly makes it possible to obtain numerically exact average results for relatively large ($L \leq 512$) aperiodic chains. On the other hand, for random chains with the binary coupling distribution there are 2^L different realizations and we performed the average over some ($N = 50\,000$) randomly chosen samples.

First, we investigate the probability distribution of the energy gap $P_L(\Delta E)$ at the critical point of the RS-chain. According to equation (5) the appropriate scaling variable is $\ln \Delta E / L^{1/2}$. Indeed, as seen in Figure 1, the accumulated probability distribution function

$$\Omega_L(\ln \Delta E) = \int_{-\infty}^{\ln \Delta E} dy \tilde{P}_L(y) \sim \tilde{\Omega}(\ln \Delta E / \sqrt{L}) \quad (8)$$

with $\tilde{P}_L(\ln \Delta E) = P_L(\Delta E)\Delta E$, has a good data collapse using this reduced variable. Considering now the same quantity for the random chain one can observe the same scaling behavior, as shown in the insert of Figure 1. Thus we can conclude, that both the random and the RS-chains have logarithmically broad distribution of the energy gaps at the critical point, from this fact one expects similar consequences for the critical behavior in the two systems.

Next we turn to consider the surface magnetization of the quantum Ising chains, which can be obtained from the formula [17]

$$m_s(L, h) = \left[1 + \sum_{l=1}^{L-1} \prod_{j=1}^l \left(\frac{h}{J_l} \right)^2 \right]^{-1/2}, \quad (9)$$

for a given realization. For one single RS-chain, starting with the letter A this expression has been evaluated exactly [10] with the following results. For $\lambda > 1$ there is a finite critical point surface magnetization, which goes to unity as $\lambda \rightarrow \infty$, whereas for $\lambda < 1$ the surface magnetization vanishes as

$$m_s(L, h_0) \sim \exp(-\text{const.} \times \sqrt{L}). \quad (10)$$

Now considering all the possible realizations of the chain at the *aperiodic* critical point equation (7) we will see, that in *typical* samples *i.e.* which occur with probability one, the surface magnetization vanishes as in equation (10), whereas there are *rare events* with a vanishing probability $P_{\text{rare}}(L) \sim L^{-\gamma}$, but with a surface magnetization of order unity. Thus the critical surface magnetization is *non-self averaging*, it is determined by the rare events,

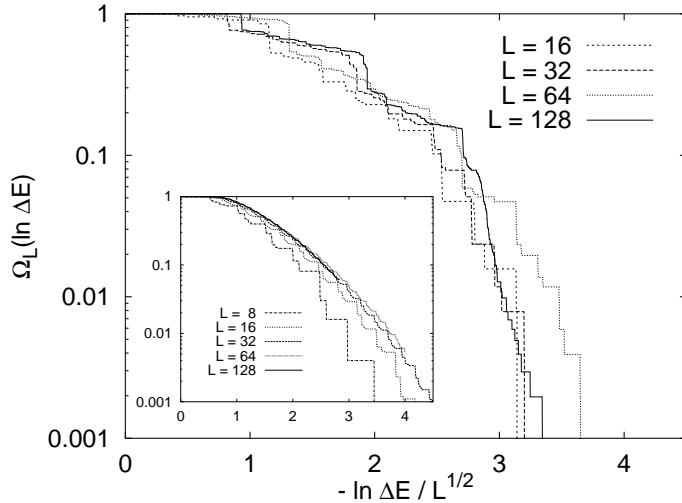


Fig. 1. Scaling plot of the accumulated probability density $\Omega(\ln \Delta E)$ versus the scaling variable $(\ln \Delta E / L^{1/2})$ for the RS sequence (exact average) with $\lambda = 4$, *cf.* equation (8). The insert shows the same for the random sequence (x and y axis as in the main figure).

and its scaling dimension x_m^s defined by the asymptotic relation $[m_s(L, h_0)]_{av} \sim L^{-x_m^s}$ is just $x_m^s = \gamma$.

In the following, using this observation, we calculate x_m^s *exactly*. First, we note that to each sample with a given distribution of the couplings one can assign a walk, which starts at the origin and takes the l -th step $+1$ (-1) for a coupling $J_l = \lambda$ ($J_l = 1/\lambda$). Then, as shown in reference [18], taking the limit $\lambda \rightarrow \infty$ only those samples have non-vanishing surface magnetization, where the corresponding walk never visits sites with negative coordinates. Thus the proportion of rare events is given by the surviving probability of the walk: $P_{rare}(L) = P_{surv}(L)$. For the random chain one should consider the random walk with $P_{surv}(L) \sim L^{-1/2}$, thus one immediately gets the exact result [3, 18, 19]:

$$x_m^s(\text{random}) = 1/2. \quad (11)$$

For the RS-chain one can perform the exact analysis [15], from which here we present the leading finite-size dependence: $[m_s(L, h_0)]_{av} = \frac{5}{8} \left(\frac{1}{\sqrt{2}} + \frac{1}{4} \right) L^{-1/2} + O(L^{-3/4})$ thus the corresponding scaling dimension

$$x_m^s(\text{RS}) = 1/2 \quad (12)$$

is the same as for the random model.

For general relevant aperiodic sequences the surface magnetization scaling dimension can be obtained by the following scaling consideration about the surviving probability of the corresponding aperiodic walk. Let us perform a discrete scale transformation, which corresponds to a substitutional step of the sequence when the length of the walks scales as $L \rightarrow LA_1$, whereas the transverse fluctuations as $y \rightarrow y|A_2|$. Then $N(L)$ the number of L -steps surviving walks from the total of different $R(L) = aL$ walks scales as $N(L) \rightarrow N(A_1L) = |A_2|N(L)$, since the number of these walks is proportional to the size of transverse fluctuations. Consequently the surviving probability $P_{surv}(L) = N(L)/R(L)$ satisfies the scaling relation

$P_{surv}(A_1L) = |A_2|/A_1 P_{surv}(L)$, with the general result

$$x_m^s = 1 - \omega. \quad (13)$$

This simple exponent relation, which is valid for the random and RS chains, has been numerically checked for the first members of the k -general chain.

Next we turn to calculate the correlation length critical exponent ν from the $\delta = \ln h$ dependence of the surface magnetization. In the scaling limit $L \gg 1$, $|\delta| \ll 1$ the surface magnetization can be written as $[m_s(L, \delta)]_{av} = [m_s(L, 0)]_{av} \tilde{m}_s(\delta L^{1/\nu})$. Expanding the scaling function into a Taylor series $\tilde{m}_s(z) = 1 + bz + O(z^2)$ one obtains for the δ correction to the surface magnetization:

$$[m_s(L, \delta)]_{av} - [m_s(L, 0)]_{av} \sim \delta L^\Theta \quad (14)$$

with $\Theta = 1/\nu - x_m^s$. This exponent can also be determined exactly in the $\lambda \rightarrow \infty$ limit from random walk arguments [18]. As shown in reference [18] the surface magnetization of *rare events* is given by:

$$m_s(L, \delta) = (1+n)^{-1/2} - \delta \frac{\sum_{i=1}^n l_i}{(n+1)^{3/2}} + O(\delta^2), \quad (15)$$

where the corresponding surviving walk returns n -times to its starting point after l_1, l_2, \dots, l_n steps. On the basis of (15) we argue that Θ is connected to the surface fractal dimension d_s of the surviving walks, defined through the asymptotic dependence of the number of return points n of a surviving walk of L steps, $n \sim L^{d_s}$. Now, to perform the average of the linear term in (15) one should take into account that from the $R(L)$ different samples there are $O(n)$, which give the most important contribution: each of those has $O(n)$ return points of characteristic lengths $l_i \sim L$. Consequently, the average of the linear term in (15) grows as $L^{d_s/2}$, thus comparing with (14) one gets the exponent relation:

$$\frac{1}{\nu} - x_m^s = \frac{d_s}{2}. \quad (16)$$

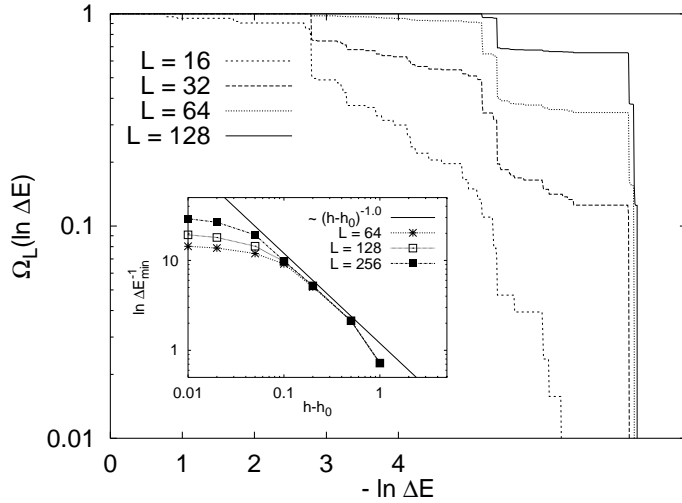


Fig. 2. The accumulated probability density $\Omega(\Delta E)$ for the RS sequence (exact average) with $\lambda = 4$ slightly above the critical point ($h = 1.5$). The distribution is chopped off at $\ln \Delta E_{\min}^{-1}(h = 1.5) \approx 7.3$. The insert shows $\ln \Delta E_{\min}^{-1}(h)$ versus the distance from the critical point ($h - h_0 \sim \delta$ for $h \rightarrow h_0$) in the RS sequence for different system sizes. The straight line has slope -1 , as predicted by (20).

The random case

$$\nu(\text{random}) = 2 \quad (17)$$

is formally contained in (16) with $d_s = 0$, since a surviving random walk returns $n = O(1)$ -times to the starting point. For the family of k -general sequences $d_s = 1/2$ for all values of k , thus the corresponding correlation length exponent is $\nu(k) = 4/(5 - 4\omega_k)$, with ω_k given in (6). In particular for the RS-sequence we get

$$\nu(\text{RS}) = 4/3, \quad (18)$$

which we also checked numerically by evaluating equation (15) exactly up to $L = 2$ [21]. Thus, by comparing (17) and (18) we conclude that the *RS and the random Ising quantum chain are not in the same universality class.*

Next we turn to study the magnetization in the bulk and calculate the scaling dimension of the bulk magnetization $x_m = \beta/\nu$ from the behavior of the average magnetization profiles at the critical point in finite systems. As will be shown in the detailed publication [15] the average magnetization profiles for the RS-chain are in excellent agreement with the conformal results [20,21], in a similar way as observed for random chains [22,23]. From the scaling behavior of the profiles x_m can be estimated as

$$x_m(\text{RS}) = 0.160 \pm 0.005, \quad (19)$$

which also differs from the random chain value $x_m(\text{random}) = (3 - \sqrt{5})/4 = 0.191$ [3].

Finally, we turn to discuss the properties of the RS-chain in the disordered phase. For the random model, as known from exact results [3,19], the susceptibility diverges in a whole region, in the so-called Griffiths-phase [24]. This non-analytical behavior is due to a broad distribution of the energy gaps, which scales in finite systems as $\Delta E(L, \delta) \sim L^{-z(\delta)}$, with the dynamical exponent $z(\delta)$ [12]. As a consequence, in the infinite chain there is no finite time-scale and the autocorrelation function decays algebraically with an exponent which is related to $z(\delta)$ [18].

For relevantly aperiodic chains the same type of scenario, *i.e.* the existence of a Griffiths-phase is speculated [6]. To clarify this issue for the RS-chain we have calculated the distribution function of the energy gap in the disordered phase. As seen in Figure 2 the accumulated distribution function for the RS-chain has a qualitatively different behavior, than for the random chain: there is an L -independent cut-off at $\Delta E_{\min}(\delta)$. As a consequence in the disordered phase the autocorrelation function always decays exponentially with a relaxation time $t_r \sim \Delta E_{\min}^{-1}(\delta)$ and the susceptibility and other physical quantities remain analytic. Therefore there is *no Griffiths-region* in the RS-chain and a similar scenario is expected to hold for any aperiodic quantum spin chain.

One can estimate the minimal energy gap $\Delta E_{\min}(\delta)$ close to critical point from the related expression in equation (5) by replacing there L with the corresponding characteristic length-scale in the off-critical region. We note, that this length-scale is not the average correlation length, since it is related to a single sample. In this case the aperiodic length scale l_{ap} is obtained [11,10] by equating the aperiodic (fluctuating) energy contribution $\sim l_{\text{ap}}^{\omega-1}$ with the “thermal” energy $\sim \delta$ giving $l_{\text{ap}} \sim \delta^{-1/(1-\omega)}$. Thus the minimal energy gap is expected to scale as

$$\Delta E_{\min}(\delta) \sim \exp(-\text{const.} \times \delta^{-\omega/(1-\omega)}). \quad (20)$$

This relation is indeed satisfied for the RS-chain, since in this case according to numerical results $\ln \Delta E_{\min}(\delta) \sim \delta^{-1}$, as can be seen in the insert of Figure 2.

To summarize, we have made a comparative study of the critical properties of random and relevantly aperiodic quantum Ising chains. At the critical point the two systems behave very similarly, some critical exponents are found even identical. This similarity is mainly attributed to the fact that, at the critical point the distribution functions of different physical quantities in the two systems qualitatively agree. Outside the critical point, where the low energy tail of the distributions is of importance, the two systems behave differently. In the random system,

with exponentially many realizations, there is no minimal energy scale, whereas in the aperiodic chain with linearly many independent realizations there exists a minimal energy cut-off. This leads then to the absence of the Griffiths phase in aperiodic systems.

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