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Critical Behavior of the Aperiodic Quantum Ising Chain in a Transverse Magnetic Field

J. M. Luck[1]

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We consider the quantum spin-1/2 Ising chain in a uniform transverse magnetic field, with an aperiodic sequence of ferromagnetic exchange couplings. This system is a limiting anisotropic case of the classical two-dimensional Ising model with an arbitrary layered modulation. Its formal solution via a Jordan–Wigner transformation enables us to obtain a detailed description of the influence of the aperiodic modulation on the singularity of the ground-state energy at the critical point. The key concept is that of the *fluctuation* of the sums of any number of consecutive couplings at the critical point. When the fluctuation is *bounded*, the model belongs to the "Onsager universality class" of the uniform chain. The amplitude of the logarithmic divergence in the specific heat is proportional to the velocity of the fermionic excitations, for which we give explicit expressions in most cases of interest, including the periodic and quasiperiodic cases, the Thue–Morse chain, and the random dimer model. When the couplings exhibit an *unbounded* fluctuation, the critical singularity is shown to be generically similar to that of the disordered chain: the ground-state energy has finite derivatives of all orders at the critical point, and an exponentially small singular part, for which we give a quantitative estimate. In the *marginal* case of a logarithmically divergent fluctuation, e.g., for the period-doubling sequence or the circle sequence, there is a negative specific heat exponent α, which varies continuously with the strength of the aperiodic modulation.

KEY WORDS: Automata and substitutions; critical phenomena; incommensurate structures; Ising model; phase transitions; quantum spin chains; quasicrystals.

1. INTRODUCTION

Since the experimental discovery of quasicrystals, intense activity has been devoted to the study of aperiodic structures in order to understand the

[1] Service de Physique Théorique (Laboratoire de la Direction des Sciences de la Matière du Commissariat à l'Énergie Atomique), Centre d'Études de Saclay, 91191 Gif-sur-Yvette Cedex, France.

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interplay between their geometrical characteristics, such as self-similarity and/or quasiperiodicity, and their physical properties. The model systems which allow for a quantitative analysis of these matters are essentially limited to the realm of one-dimensional structures, i.e., aperiodic chains. This relationship between geometrical and physical properties has been mostly explored so far in the context of linear problems, such as lattice dynamics (phonon spectra) or electronic spectra (tight-binding or Kronig–Penney Hamiltonians) (see refs. 1 and 2 for recent reviews). Many specific results have been established for models based, e.g., on the Fibonacci sequence or the Thue–Morse sequence. Some generic results are also available. Focusing our attention onto the tight-binding Hamiltonian, let us mention mathematical results about gap labeling theorems,[3,4] which tell us about the possible discrete values taken by the integrated density of states in gaps of, e.g., electronic spectra. It turns out that all the gaps are generically open in one dimension. The scaling behavior of the gap widths as a function of the strength of the aperiodic modulation has been related in a quantitative way[5] to the behavior of the Fourier transform of the potential at the corresponding wavevector.

Less is known about the physical properties described by nonlinear equations, such as the spin systems which model magnetic properties. A prototype of such systems is provided by the quantum Ising chain in a transverse field. The aim of the present work is to study the influence of an aperiodic modulation on the critical behavior of the model. This can be done in a detailed way, because the model is formally solvable by means of a Jordan–Wigner transformation.[6]

The quantum spin-1/2 Ising chain in a transverse magnetic field is defined by the Hamiltonian

$$\mathscr{H} = -\sum_n J_n \sigma_n^{(1)} \sigma_{n+1}^{(1)} - h \sum_n \sigma_n^{(3)} \tag{1.1}$$

Every site n of the chain is occupied by a spin-1/2 operator with components $\sigma_n^{(a)}$ ($a = 1, 2, 3$), equal to half the Pauli matrices. The constant $h > 0$ denotes the transverse magnetic field, whereas the ferromagnetic exchange couplings $J_n > 0$ between pairs of nearest neighbors form an arbitrary infinite sequence. We introduce for further reference dimensionless couplings ε_n and δ_n through

$$\varepsilon_n = \exp \delta_n = \frac{J_n}{2h} \tag{1.2}$$

It was realized long ago[7] that the quantum chain described by the Hamiltonian (1.1) at zero temperature can be viewed as a very anisotropic

limit of the two-dimensional classical Ising model at finite temperature $T = 1/\beta$ in zero external field, described by the Hamiltonian

$$H_{2D} = -\sum_{m,n} (K_{1,n} S_{m,n} S_{m,n+1} + K_2 S_{m,n} S_{m+1,n}) \tag{1.3}$$

where the $S_{m,n} = \pm 1$ are now classical Ising spins, living on the sites of a "rectangular" lattice. The couplings $K_{1,n}$ in the "spacelike" direction depend on n, whereas the coupling K_2 in the "timelike" direction is uniform. The correspondence between both models is as follows: the quantum problem is the limit of the classical one as $K_{1,n} \to 0$ and $K_2 \to +\infty$, so that $\beta K_{1,n} = \varepsilon_n \exp(-2\beta K_2)$. Let us emphasize that the modulation of the classical model is *layered*, namely, that the couplings depend only on one lattice coordinate n.

In the following, we will use the language of the ground-state properties of the quantum spin chain, for the sake of simplicity. Our results can be translated, *mutatis mutandis*, in terms of finite-temperature properties of the classical two-dimensional Ising model. Since the original solution by Onsager[8] of the two-dimensional Ising model, many alternative approaches have been proposed, which explains why this model can be solved exactly. One of the most fruitful methods has been introduced by Lieb *et al.*[6] This general approach consists in an exact mapping of the Hamiltonian of the spin chain onto a model of free fermions, by means of a Jordan–Wigner transformation, introducing fermionic operators which are nonlocal in the original spin degrees of freedom. This transformation works for the general Hamiltonian (1.1), with an arbitrary sequence of exchange couplings. Dtails will be given in Section 2.1.

The two-dimensional Ising model with layered quenched disorder, where the exchange couplings $K_{1,n}$ are independent random variables, has been studied in refs. 9–12. The most remarkable outcome of this analysis is that the Onsager critical singularity of the uniform Ising model (the well-known logarithmic divergence of the specific heat) is turned by an arbitrarily small disorder into an exponentially small essential singularity for the free energy, which has finite derivatives of any order at the critical temperature.

The fact that any amount of quenched disorder alters the critical singularity can be understood by means of the following scaling argument, which applies to any aperiodic sequence $\{J_n\}$ of exchange couplings, generalizing thus the *Harris criterion.*[13] We will show in Section 2.3 that the critical point is defined by the condition $\mu = 0$, where μ denotes the following Cesàro average:

$$\mu = \overline{\delta_n} \equiv \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \delta_n \tag{1.4}$$

of the δ_n defined in Eq. (1.2). In other words, for any physically "reasonable" sequence of exchange couplings, there is a finite critical value of the magnetic field, namely

$$h_c = \tfrac{1}{2} \exp(\overline{\ln J_n}) \tag{1.5}$$

so that

$$\mu = \ln \frac{h_c}{h} \tag{1.6}$$

is a measure of the distance to criticality [$\mu \approx -(h - h_c)/h_c$ as $h \to h_c$].

As it turns out, the key concept is that of the *fluctuation* of the exchange couplings. Consider a finite sample of the chain, consisting of N spins ($1 \leqslant n \leqslant N$). We *define* the associated fluctuation g_N as the following partial sum of the reduced couplings δ_n at criticality:

$$g_N = \sum_{n=1}^{N} \delta_n \tag{1.7}$$

The analogous concept of the fluctuation of the atomic positions in a structure w.r.t. its underlying average lattice has proved to be fruitful in the study of the types of order present in aperiodic structures.[14–17]

In virtue of the criticality condition $\mu = 0$, the fluctuation cannot be "large," in the sense that we have $g_N \ll N$ for large N. Nevertheless, because of its finiteness, the sample will not be exactly at criticality, but rather at a small distance to the critical point, which can be estimated as $\mu \sim g_N/N$. On the other hand, it is well known that the uniform chain has a correlation length which diverges as $\xi \sim \mu^{-\nu}$, with $\nu = 1$. The aperiodic modulation will be *relevant*, using the language of the renormalization group, i.e., the nature of the critical singularity will be altered, if the shift of the critical coupling induced by the finite size of the sample is (much) larger than the value of μ for which the correlation length ξ is comparable to the sample size N, i.e., $\mu \sim 1/N$. Both above estimates imply that the relevance condition reads $g_N \gg 1$.

We conclude from the above heuristic argument that any unbounded fluctuation in the sequence of exchange couplings drives the model out of the "Onsager universality class," so that the critical singularity is weaker than that of the uniform chain.

The aim of this paper is to make this prediction more quantitative, and to relate the nature of the critical singularity of the ground-state energy to the asymptotic growth of the fluctuation of the exchange couplings. Some previous works have already led to partial results on these matters.

Several authors[18–21] have shown that the Fibonacci quantum Ising chain, where the exchange couplings follow the quasiperiodic ordering of the Fibonacci sequence, is in the Onsager universality class, in agreement with the above criterion. The value of the prefactor of the logarithmic divergence of the specific heat has also been derived. These results have been generalized in several respects.[22–29] It is shown in refs. 30 and 31 that, among the deterministic self-similar structures, only those for which the sequence of exchange couplings has a bounded fluctuation belong to the "Onsager universality class." More precisely, the authors of ref. 31 suggest that "the behavior is similar to the random case" whenever the fluctuation g_N is unbounded. All these results are in accord with the generalized Harris criterion exposed above. A more thorough analysis is performed hereafter, which yields quantitative predictions.

The remainder of this article is as follows. In Section 2, we recall some general formalism about the Jordan–Wigner transformation, and we derive the prefactor of the critical singularity for any periodic chain. In Section 3, we present a scaling analysis of the critical region of the disordered case, recovering thus most outcomes of refs. 9 and 12 in an elementary and more accurate fashion. The subsequent sections present our main novel results concerning the critical singularity when the exchange couplings follow an arbitrary sequence. The case of a bounded fluctuation, yielding an Onsager-like singularity, is described in Section 4, whereas Section 5 deals with the weaker critical singularities induced by unbounded fluctuations. Among other results, the marginal case of a logarithmically growing fluctuation is shown to yield a continuously varying specific heat exponent $\alpha < 0$.

2. PERIODIC CHAINS

2.1. Generalities

The quantum Ising chain defined by the Hamiltonian (1.1) is exactly solvable for an arbitrary sequence of exchange constants $\{J_n\}$, in the sense that it can be mapped onto a free fermionic field, by means of a Jordan–Wigner transformation. In the context of quantum spin chains, this well-known procedure was initiated long ago,[6] as recalled in the Introduction. Assume for definiteness that the chain is finite and is made of N spins ($1 \leqslant n \leqslant N$), with prescribed boundary conditions. Define at each site the raising and lowering operators

$$a_n^\dagger = \sigma_n^{(1)} + i\sigma_n^{(2)}, \qquad a_n = \sigma_n^{(1)} - i\sigma_n^{(2)} \tag{2.1}$$

We have then $\sigma_n^{(3)} = a_n^\dagger a_n - 1/2$, so that the Hamiltonian (1.1) can be written as a quadratic form. The Jordan–Wigner transformation consists in introducing the nonlocal operators

$$c_n = \exp\left(i\pi \sum_{m=1}^{n-1} a_m^\dagger a_m \right) a_n, \qquad c_n^\dagger = a_n^\dagger \exp\left(-i\pi \sum_{m=1}^{n-1} a_m^\dagger a_m \right) \tag{2.2}$$

which obey the anticommutation relations of annihilation and creation operators of independent fermions. The Hamiltonian (1.1) can be recast as

$$\mathcal{H} = -h \sum_n \left(c_n^\dagger c_n - \frac{1}{2} \right) - \sum_n \frac{J_n}{4} (c_n^\dagger - c_n)(c_{n+1}^\dagger + c_{n+1}) \tag{2.3}$$

The last step consists in diagonalizing the quadratic form (2.3) by means of a Bogoliubov transformation, of the form

$$\begin{aligned} \eta_\alpha &= \tfrac{1}{2} \sum_n \left[(\phi_{\alpha,n} + \psi_{\alpha,n}) c_n + (\phi_{\alpha,n} - \psi_{\alpha,n}) c_n^\dagger \right] \\ \eta_\alpha^\dagger &= \tfrac{1}{2} \sum_n \left[(\phi_{\alpha,n} + \psi_{\alpha,n}) c_n^\dagger + (\phi_{\alpha,n} - \psi_{\alpha,n}) c_n \right] \end{aligned} \tag{2.4}$$

The Hamiltonian of the spin chain thus takes the following form:

$$\mathcal{H} = h \sum_{\alpha=1}^{N} \Lambda_\alpha (\eta_\alpha^\dagger \eta_\alpha - \tfrac{1}{2}) \tag{2.5}$$

The dimensionless excitation energies $\Lambda_\alpha > 0$ and the coefficients $\{\phi_{\alpha,n}, \psi_{\alpha,n}\}$ of the Bogoliubov transformation (2.4) are the generalized eigenvalues and eigenvectors of the following linear difference equations:

$$\begin{aligned} \Lambda \psi_n &= -\phi_n - \varepsilon_{n-1} \phi_{n-1} \\ \Lambda \phi_n &= -\psi_n - \varepsilon_n \psi_{n+1} \end{aligned} \tag{2.6}$$

where the reduced exchange couplings ε_n have been introduced in Eq. (1.2). The system (2.6) has exactly N eigenvalues on the finite chain, with prescribed boundary conditions inherited from the spin problem.

The quantum ground state of the finite chain is the state $|\Omega\rangle$, which is annihilated by all the η_α. Its energy reads

$$E_0 = -\frac{h}{2} \sum_{\alpha=1}^{N} \Lambda_\alpha \tag{2.7}$$

As a consequence, the thermodynamic reduced ground-state energy $\mathscr{E}$ per spin is

$$\mathscr{E} = \lim_{N \to \infty} \frac{E_0}{Nh} = -\frac{1}{2} \int_0^\infty \Lambda \rho(\Lambda)\, d\Lambda \tag{2.8}$$

where a factor of h has been taken out in order for $\mathscr{E}$ to be dimensionless.

In Eq. (2.8), $\rho(\Lambda)$ denotes the normalized density of states of the spectral problem (2.6), defined formally as

$$\rho(\Lambda) = \lim_{N \to \infty} \frac{1}{N} \sum_{\alpha=1}^{N} \delta(\Lambda - \Lambda_\alpha) \tag{2.9}$$

The spectrum of the Hamiltonian $\mathscr{H}$ exhibits the following energy gap between its ground state and its first one-fermion excited state:

$$(E_1 - E_0)_{\min} = h\Lambda_{\min} \tag{2.10}$$

where $\Lambda_{\min} \geqslant 0$ is the lower bound of the support of the density of states.

It is advantageous to recast Eq. (2.6) into the following forms, which are more familiar in the context of physical properties of inhomogeneous chains. First, it is equivalent to either one of the following second-order (three-term) equations, involving the $\{\psi_n\}$ or the $\{\phi_n\}$:

$$\begin{aligned} \Lambda^2 \psi_n &= (1 + \varepsilon_{n-1}^2)\psi_n + \varepsilon_n \psi_{n+1} + \varepsilon_{n-1}\psi_{n-1} \\ \Lambda^2 \phi_n &= (1 + \varepsilon_n^2)\phi_n + \varepsilon_n \phi_{n+1} + \varepsilon_{n-1}\phi_{n-1} \end{aligned} \tag{2.11}$$

The system (2.6) can alternatively be rewritten in the following matrix form:

$$\begin{pmatrix} \phi_{n+1} \\ \psi_{n+1} \end{pmatrix} = \mathscr{T}_n \begin{pmatrix} \phi_n \\ \psi_n \end{pmatrix} \tag{2.12}$$

where the $\mathscr{T}_n$ are 2×2 transfer matrices, with unit determinant, which read

$$\mathscr{T}_n = \frac{1}{\varepsilon_n} \begin{pmatrix} \Lambda^2 - \varepsilon_n^2 & \Lambda \\ -\Lambda & -1 \end{pmatrix} \tag{2.13}$$

The following expression of the commutator of the transfer matrices pertaining to two different bonds

$$[\mathscr{T}_m, \mathscr{T}_n] = \Lambda \frac{\varepsilon_n^2 - \varepsilon_m^2}{\varepsilon_m \varepsilon_n} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.14}$$

shows that these matrices commute among themselves for the special value $\Lambda = 0$ of the fermionic energy. This observation will be the starting point of the perturbative analysis performed in Section 2.3.

2.2. The Uniform Chain

The above formalism easily yields the well-known Onsager solution in the case of a uniform chain. In this situation, where the ε_n have the constant value ε, the excitation energies $\Lambda(q)$ depend on a Bloch momentum q. The dispersion relation which relates q and Λ can be obtained from the transfer matrix as $\operatorname{tr} \mathscr{T} = -2\cos q$, where a minus sign has been inserted conventionally, in order to have $q = 0$ at the bottom of the spectrum. We thus obtain

$$\Lambda^2 = 1 - 2\varepsilon \cos q + \varepsilon^2 = (1-\varepsilon)^2 + 4\varepsilon \sin^2(q/2) \tag{2.15}$$

This relation shows that the spectrum of fermionic energies consists of a single band, namely the interval $S = [|\varepsilon - 1|, \varepsilon + 1]$.

The reduced ground-state energy is given by

$$\mathscr{E} = -\frac{1}{2}\int_0^\pi \frac{dq}{\pi}(1 - 2\varepsilon\cos q + \varepsilon^2)^{1/2} = -\frac{1+\varepsilon}{\pi}\mathbf{E}(k) \tag{2.16}$$

where $\mathbf{E}(k)$ denotes the complete elliptic integral of the second kind (ref. 32, Vol. II), with modulus $k^2 = 4\varepsilon/(1+\varepsilon)^2 = 1 - \tanh^2(\mu/2)$, where μ has been introduced in Eq. (1.4).

The expression (2.16) has one isolated singularity, due to small values of q, for $\varepsilon = 1$, i.e., $J = 2h$, or equivalently $\mu = 0$. These conditions therefore define the critical point of the model. It is also worth noticing that the reduced energy gap $\Lambda_{\min} = |\varepsilon - 1| \approx |\mu|$ vanishes linearly with the distance to the critical point.

In the critical region ($\mu \to 0$), the ground-state energy has the following behavior:

$$\mathscr{E} = -\frac{1}{\pi}\left[2 + \mu + \frac{\mu^2}{8}\left(\ln\frac{64}{\mu^2} - 1\right) + \cdots\right] \tag{2.17}$$

The singular expansion (2.17) shows that the second derivative $\mathscr{C} = -\partial^2\mathscr{E}/\partial\mu^2$, which is the quantum analog of the specific heat of the two-dimensional classical Ising model, exhibits a logarithmic divergence, of the form $\mathscr{C} \approx (1/4\pi)\ln(1/\mu^2)$, which is characteristic of the "Onsager universality class."

2.3. The Critical Singularity of Periodic Chains

In this section, we consider the case where the exchange constants form any periodic array, with period M. In other terms, the chain is a periodic "crystal," with a unit cell consisting of M arbitrary couplings $\{\varepsilon_1, \ldots, \varepsilon_M\}$.

More precisely, we will perform a perturbative analysis of the bottom of the fermionic spectrum, which governs the critical behavior of the model. The starting point of this study is the observation that the commutator evaluated in Eq. (2.14) vanishes for $\Lambda = 0$. It can therefore be expected that a simplification occurs there, somehow. It will indeed turn out that the wavefunctions ϕ_n and ψ_n admit an expansion in powers of Λ. The results derived below will be used in the scaling analysis presented in Sections 4 and 5. The expression (2.27) for the velocity of fermionic excitations on an arbitrary periodic pattern seems to have been derived for the first time in ref. 11, in the context of the classical two-dimensional model. This result has been used in refs. 19 and 30, whereas refs. 20, 22, 24, and 27 also describe perturbative approaches, somehow similar to the present one.

Let us assume that ϕ_0 and ψ_0 are given. For $\Lambda = 0$, both equations of the system (2.6) are decoupled, so that we have the solution

$$\phi_n^{(0)} = \phi_0 (-1)^n \varepsilon_0 \cdots \varepsilon_{n-1}, \qquad \psi_n^{(0)} = \psi_0 \frac{(-1)^n}{\varepsilon_0 \cdots \varepsilon_{n-1}} \tag{2.18}$$

For Λ small, we expand the wavefunctions as the following power series:

$$\begin{aligned} \phi_n &= \phi_n^{(0)} + \phi_n^{(1)} \Lambda + \phi_n^{(2)} \Lambda^2 + \cdots \\ \psi_n &= \psi_n^{(0)} + \psi_n^{(1)} \Lambda + \psi_n^{(2)} \Lambda^2 + \cdots \end{aligned} \tag{2.19}$$

The first-order terms are determined by the recursion equations

$$\begin{aligned} \phi_n^{(1)} + \varepsilon_{n-1} \phi_{n-1}^{(1)} &= -\psi_n^{(0)} \\ \psi_n^{(1)} + \varepsilon_n \psi_{n+1}^{(1)} &= -\phi_n^{(0)} \end{aligned} \tag{2.20}$$

from which we obtain

$$\begin{aligned} \phi_n^{(1)} &= (-1)^{n-1} \psi_0 \sum_{k=1}^{n} \frac{\varepsilon_k \cdots \varepsilon_{n-1}}{\varepsilon_0 \cdots \varepsilon_{k-1}} \\ \psi_n^{(1)} &= (-1)^n \phi_0 \sum_{k=0}^{n-1} \frac{\varepsilon_0 \cdots \varepsilon_{k-1}}{\varepsilon_k \cdots \varepsilon_{n-1}} \end{aligned} \tag{2.21}$$

The second-order terms are determined by the recursion equations

$$\begin{aligned} \phi_n^{(2)} + \varepsilon_{n-1}\phi_{n-1}^{(2)} &= -\psi_n^{(1)} \\ \psi_n^{(2)} + \varepsilon_n \psi_{n+1}^{(2)} &= -\phi_n^{(1)} \end{aligned} \tag{2.22}$$

from which we obtain

$$\begin{aligned} \phi_n^{(2)} &= -\phi_n^{(0)} S_1(n), \qquad \text{with} \quad S_1(n) = \sum_{k=1}^{n} \sum_{l=0}^{k-1} \frac{1}{\varepsilon_l^2 \cdots \varepsilon_{k-1}^2} \\ \psi_n^{(2)} &= -\psi_n^{(0)} S_2(n), \qquad \text{with} \quad S_2(n) = \sum_{k=1}^{n-1} \left(1 + \sum_{l=1}^{k-1} \varepsilon_l^2 \cdots \varepsilon_{k-1}^2 \right) \end{aligned} \tag{2.23}$$

The above expansion can be recast in matrix form

$$\begin{pmatrix} \phi_M \\ \psi_M \end{pmatrix} = \mathscr{T}_{\text{cell}} \begin{pmatrix} \phi_0 \\ \psi_0 \end{pmatrix} \tag{2.24}$$

where $\mathscr{T}_{\text{cell}}$ is the transfer matrix which describes the propagation across one unit cell. We can derive from this expression an approximate dispersion relation of the fermionic excitations for Λ small, in the form

$$\begin{aligned} 2\cos(Mq) = (-1)^M \operatorname{tr} \mathscr{T}_{\text{cell}} &\approx \varepsilon_1 \cdots \varepsilon_M [1 - \Lambda^2 S_1(M)] \\ &+ \frac{1}{\varepsilon_1 \cdots \varepsilon_M} [1 - \Lambda^2 S_2(M)] \end{aligned} \tag{2.25}$$

In order to exhibit the physical meaning of this result, we introduce the following two parameters:

$$\mu = \frac{1}{M} \ln(\varepsilon_1 \cdots \varepsilon_M) = \frac{1}{M} \sum_{m=1}^{M} \delta_m \tag{2.26}$$

in agreement with Eq. (1.4), and

$$\frac{1}{v^2} = \frac{1}{M^2} \sum_{m=1}^{M} \sum_{k=1}^{M} \varepsilon_{m+1}^2 \cdots \varepsilon_{m+k}^2 \tag{2.27}$$

so that the dispersion relation (2.25) assumes the form

$$\Lambda^2 \approx v^2 (q^2 + \mu^2) \tag{2.28}$$

in the scaling region where Λ, q, and μ are small. The reduced energy gap reads

$$\Lambda_{\min} \approx v\,|\mu| \tag{2.29}$$

and the critical point corresponds to $\mu = 0$, namely

$$\varepsilon_1 \cdots \varepsilon_M = 1, \qquad \text{i.e.,} \quad \sum_{m=1}^{M} \delta_m = 0 \tag{2.30}$$

The simple form of this last result shows that the critical point of the spin chain with an arbitrary sequence of exchange couplings reads $\mu = 0$, as already announced in the Introduction, where μ has been introduced in Eq (1.4).

Going back to the periodic case, we observe that the long-wavelength fermions have the following massless relativistic dispersion law at criticality:

$$\Lambda \approx vq \tag{2.31}$$

where it is understood that v is evaluated under the criticality condition (2.30). This value of v thus represents the velocity of the massless fermionic excitations.

Finally, the critical singular part $\mathscr{E}_{sg}$ of the ground-state energy for $\mu \to 0$ is governed by the low-lying fermionic energies, of order $\Lambda \sim \mu$, for which the relation (2.28) holds. We can therefore write the estimate

$$\mathscr{E}_{sg} \approx -\frac{v}{2} \int_0^Q \frac{dq}{\pi} (q^2 + \mu^2)^{1/2} \tag{2.32}$$

where Q is a cutoff momentum of order unity. We thus obtain

$$\mathscr{E}_{sg} \approx -\frac{v}{8\pi} \mu^2 \ln \frac{Q^2}{\mu^2} \tag{2.33}$$

This result shows that the velocity v of the fermionic excitations governs the amplitude of the critical singularity of the ground-state energy, and hence that of the logarithmic divergence of the specific heat, in the case of an arbitrary periodic chain. We recall that the expression of v has been obtained in Eq. (2.27) for any periodic chain. This general result implies $0 < v \leqslant 1$, the upper bound $v = 1$ being reached if, and only if, the chain is uniform. The result (2.17) is thus recovered (with $Q^2 = 64/e$).

We end up this section by considering the simplest nontrivial example of a periodic binary chain, with period two. We denote by Δ the strength of the periodic modulation, so that we have $\varepsilon_1 = \exp(\Delta/2)$, and $\varepsilon_2 = \exp(-\Delta/2)$ at criticality. Then yields Eq. (2.27)

$$v = \frac{1}{\cosh(\Delta/2)} \tag{2.34}$$

As expected, the velocity assumes its maximal value $v=1$ in the situation of the uniform chain ($\Delta=0$), whereas it vanishes exponentially for a large modulation.

The results derived in this section are similar to those of ref. 11, which concern the classical two-dimensional layered Ising model. Let us emphasize that the present situation yields a much simpler expression for the velocity v of fermionic excitations.

3. RANDOM CHAINS

This section is devoted to the case of disordered chains, where the reduced exchange couplings ε_n are independent random variables, with a common probability distribution. This situation is equivalent to the classical two-dimensional Ising model with layered randomness, which has been studied extensively.[9–12] We will present an exact scaling analysis of the critical region in the weak-disorder regime. Among other outcomes, we will obtain the closed-form expression (3.65) for the absolute prefactor of the critical singularity, which had not been fully understood in previous works. Moreover, besides its own interest, this approach will be used as a test case for the heuristic scaling arguments developed in Section 5.

3.1. Generalities

In the following, we make use of the formalism of the invariant measure and of the complex characteristic exponent.[5, 33–36] Let us summarize the main equations of this standard approach to the study of spectral problems related to one-dimensional random systems. We start by introducing the following Riccati variables:

$$R_n = -\frac{\varepsilon_n \psi_{n+1}}{\psi_n} = 1 + \Lambda \frac{\phi_n}{\psi_n} \tag{3.1}$$

which obey a nonlinear recursion formula

$$R_n = 1 + \varepsilon_n^2 - \Lambda^2 - \frac{\varepsilon_n^2}{R_{n-1}} \tag{3.2}$$

as a consequence of Eqs. (2.6), (2.11).

The Riccati variables R_n are asymptotically distributed, for n large, according to a stationary probability law, which is invariant under the transformation (3.2). Throughout the following, we denote by double brackets $\langle\langle \cdots \rangle\rangle$ averages w.r.t. this invariant probability measure.

We consider the recursion (3.2) for complex values of the variable Λ, and define a complex *characteristic exponent* $\Omega(\Lambda)$ by

$$\Omega(\Lambda) = \left\langle\!\!\left\langle \ln\left(-\frac{\psi_{n+1}}{\psi_n}\right)\right\rangle\!\!\right\rangle = \langle\!\langle \ln R_n \rangle\!\rangle - \mu \tag{3.3}$$

where μ has been introduced in Eq. (1.4).

When Λ goes to the real axis, we split the characteristic exponent into its real and imaginary parts, according to

$$\Omega(\Lambda \pm i0) = \gamma(\Lambda) \pm i\pi H(\Lambda) \tag{3.4}$$

These quantities have the following interpretation[33–36]:

1. The *Lyapunov exponent* $\gamma(\Lambda) > 0$ describes the mean exponential falloff of a generic normalizable eigenfunction (ϕ_n, ψ_n) with energy Λ:

$$\phi_n \sim \psi_n \sim \exp[-\gamma(\Lambda)\,|n|] \tag{3.5}$$

In other words, the typical extent of the fermionic eigenstates is given by the localization length $\xi(\Lambda) = 1/\gamma(\Lambda)$.

2. The *integrated density of states* $H(\Lambda)$ represents the fraction of the excitation energies Λ_α lying below Λ, defined as [see Eq. (2.9)]

$$H(\Lambda) = \int_0^\Lambda \rho(\Lambda')\, d\Lambda' = \lim_{N\to\infty} \frac{1}{N} \#\{\Lambda_\alpha < \Lambda\} \tag{3.6}$$

The properties recalled above can be demonstrated by means of the following expression:

$$\psi_n = (-1)^n \frac{R_0 \cdots R_{n-1}}{\varepsilon_0 \cdots \varepsilon_{n-1}} \psi_0 \tag{3.7}$$

The interpretation of the Lyapunov exponent $\gamma(\Lambda)$ as an inverse localization length is rather straightforward, whereas the connection with the integrated density of states is established via the following Sturm oscillation property. Consider a finite sample, made of N spins, and assume that the excitation energies are ordered as $\Lambda_1 < \cdots < \Lambda_N$. Then the wavefunctions ϕ_n or ψ_n of the fermionic eigenstate number α $(1 \leqslant \alpha \leqslant N)$ have exactly $(N-\alpha)$ nodes, i.e., $(N-\alpha)$ sign changes. As a consequence, among the N corresponding Riccati variables, $(N-\alpha)$ are positive and α are negative.

We end up this introductory section by noticing that the explicit formulas (2.18) for the wavefunctions ϕ_n and ψ_n for $\Lambda = 0$ imply that we have

$$\Omega(\Lambda = 0) = |\mu| \tag{3.8}$$

This simple and general result confirms that the critical point $\mu = 0$ is a singular point, as already announced in the Introduction, and shown in Section 2.3 via another approach. Indeed, the characteristic exponent Ω is not differentiable w.r.t. μ at criticality ($\mu = 0$) at the bottom of the fermionic spectrum ($\Lambda = 0$), irrespective of the nature of the exchange couplings. Moreover, the localization length $\xi(\Lambda = 0)$ is infinite at criticality.

3.2. Weak-Disorder Expansion

In the following, we shall be mostly interested in the critical region and in the weak-disorder regime. The distribution of the random exchange couplings will therefore only enter the analysis through its first two moments, namely

$$\overline{\delta_n} = \mu, \qquad \overline{\delta_n^2} = \mu^2 + \Delta^2 \tag{3.9}$$

The average μ, defined in Eq. (1.4), is a measure of the distance to criticality, as explained in the Introduction, whereas the r.m.s. deviation Δ represents the strength of disorder. Both parameters μ and Δ are assumed to be small throughout the rest of Section 3.

In order to study the influence of quenched disorder on the critical behavior of the Ising chain, the most direct approach consists in performing a weak-disorder expansion of the characteristic exponent Ω, along the lines of refs. 5, 33, and 34. It is advantageous to perform this expansion for a complex fermionic energy Λ, outside the spectrum. Moreover, it will be sufficient for the present purpose to consider the critical region ($\mu \to 0$).

The starting point of the analysis is the following. At criticality and without disorder, we have $\delta_n = 0$, i.e., $\varepsilon_n = 1$, so that the recursion (3.2) between Riccati variables reads

$$R_n = 2 - \Lambda^2 - \frac{1}{R_{n-1}} \tag{3.10}$$

The fixed points of the above transformation are $R = e^t$ (attractive, stable), and $R = e^{-t}$ (repulsive, unstable), where we have set

$$\Lambda^2 = 2(1 - \cosh t) = -4 \sinh^2 \frac{t}{2} \qquad (\mathrm{Re}\, t > 0,\ |\mathrm{Im}\, t| < \pi) \tag{3.11}$$

We thus get

$$\Omega = t \tag{3.12}$$

In order to generate a systematic expansion of the characteristic exponent around its value (3.12), we perform the change of variable

$$R_n = \frac{e^{-t}Y_n - e^t}{Y_n - 1}, \qquad Y_n = \frac{R_n - e^t}{R_n - e^{-t}} \tag{3.13}$$

The new random variables Y_n obey the recursion

$$Y_n = \frac{e^{-2t}Y_{n-1} + a_n(1 + e^{-t}Y_{n-1})}{1 + a_n(1 + e^{-t}Y_{n-1})} \tag{3.14}$$

with the notation

$$a_n = \frac{\varepsilon_n^2 - 1}{1 + e^t} \tag{3.15}$$

and the characteristic exponent is expressed as

$$\Omega = t - \mu + \left\langle\!\!\left\langle \ln \frac{1 - e^{-2t}Y_n}{1 - Y_n} \right\rangle\!\!\right\rangle \tag{3.16}$$

or equivalently,

$$\Omega = t - \mu + \langle\!\langle \ln[1 + a_n(1 + e^{-t}Y_{n-1})] \rangle\!\rangle \tag{3.17}$$

Let us now derive the expansion of Ω up to second order in μ and Δ. To do so, we expand Eq. (3.17) up to second order in the a_n, anticipating the behavior $Y_n \sim a_n$. We thus obtain

$$\Omega = t - \mu + \overline{a_n} + e^{-t}\overline{a_n}\langle\!\langle Y_{n-1} \rangle\!\rangle - \tfrac{1}{2}\overline{a_n^2} + \cdots \tag{3.18}$$

On the other hand, by expanding the recursion (3.14) up to first order, we get

$$Y_n = e^{-2t}Y_{n-1} + a_n + \cdots \tag{3.19}$$

so that

$$\langle\!\langle Y_{n-1} \rangle\!\rangle = \frac{\overline{a_n}}{1 - e^{-2t}} \tag{3.20}$$

and

$$\Omega = t - \mu + \overline{a_n} + \frac{1}{2\sinh t}\overline{a_n}^2 - \frac{1}{2}\overline{a_n^2} + \cdots \tag{3.21}$$

Then, by expanding the definition (3.15), we get

$$\overline{a_n} = \frac{2}{1+e^t}(\mu + \mu^2 + \Delta^2 + \cdots), \qquad \overline{a_n^2} = \frac{4}{(1+e^t)^2}(\mu^2 + \Delta^2 + \cdots) \tag{3.22}$$

The final outcome of this analysis is

$$\Omega = t - \tau\mu + \frac{1-\tau^2}{2}\Delta^2 + \frac{1-\tau^4}{4\tau}\mu^2 + \cdots \tag{3.23}$$

with the notation

$$\tau = \tanh\frac{t}{2} \tag{3.24}$$

It is worth noticing that the successive terms of the weak-disorder expansion (3.23) are more and more singular near the bottom of the spectrum ($-\Delta^2 \approx t^2 \approx 4\tau^2 \to 0$).

3.3. Scaling Laws and Critical Behavior

The last observation suggests the existence of a nontrivial scaling behavior when t, μ, and Δ^2 go simultaneously to zero at the same scale. A quantitative study of this regime is the purpose of the present section. We set

$$x = \frac{t}{\Delta^2}, \qquad y = \frac{\mu}{\Delta^2} \tag{3.25}$$

and our aim is to show that the characteristic exponent Ω obeys a scaling law of the form

$$\Omega \approx \Delta^2 F(x, y) \tag{3.26}$$

in the weak-disorder regime ($\Delta \to 0$), keeping the scaling variables x (complex) and y (real) fixed, so that one is driven to the bottom of the fermionic spectrum ($t \to 0$) and to criticality ($\mu \to 0$). We recall the hypothesis $\mathrm{Re}\, t > 0$, made in the definition (3.11), implying $\mathrm{Re}\, x > 0$. The fermionic spectrum can be reached via the analytic continuation to $t \approx i\Delta$.

The starting point of the analysis consists in expanding the recursion relation (3.14) to second order in a_n. We thus obtain

$$e^{2t} Y_n = Y_{n-1} + (1 - Y_{n-1}^2) a_n + (Y_{n-1} + 1)(Y_{n-1}^2 - 1) a_n^2 + \cdots \tag{3.27}$$

where we have already set $t=0$ in the coefficients in the r.h.s. To the same order, Eq. (3.27) implies the following recursion relations:

$$e^{2mt}d_m = d_m + m(\overline{a_n^2} - \overline{a_n})(d_{m+1} - d_{m-1}) + \frac{m}{2}\overline{a_n^2}[(m+1)d_{m+2} + (m-1)d_{m-2} - 2md_m] \tag{3.28}$$

among the moments of the invariant measure

$$d_m = \langle\langle Y_n^m \rangle\rangle \tag{3.29}$$

In the scaling region, the expressions (3.22) simplify to $\overline{a_n} = (y+1)\Delta^2$, and $\overline{a_n^2} = \Delta^2$, whereas higher-order moments are subleading. As a consequence, Eq. (3.28) takes the following limit form:

$$4xd_m = 2y(d_{m-1} - d_{m+1}) + (m+1)d_{m+2} + (m-1)d_{m-2} - 2md_m \tag{3.30}$$

and the expression (3.17) of the characteristic exponent yields the scaling form (3.26), with

$$F(x, y) = x + yd_1 + \tfrac{1}{2}(1 - d_2) \tag{3.31}$$

The determination of the scaling function $F(x, y)$ thus amounts to finding the scaling forms d_1 and d_2 of the first two moments of the invariant measure. This can be done as follows. We introduce the generating function of the moments d_m, namely

$$f(z) = \sum_{m \geqslant 1} d_m z^m = \left\langle\!\!\left\langle \frac{zY_n}{1 - zY_n} \right\rangle\!\!\right\rangle \tag{3.32}$$

The recursion relation (3.30) is equivalent to the following first-order linear differential equation for $f(z)$:

$$(1-z^2)^2 z \frac{df}{dz} + [-4xz^2 - 2yz(1-z^2) + z^4 - 1]f = z^2[d_2 - z^2 - 2y(d_1 + z)] \tag{3.33}$$

This equation can be solved by "varying the constant." To do so, we first solve the homogeneous equation, obtained by setting the r.h.s. of Eq. (3.33) equal to zero. The solution reads

$$f_0(z) = C \frac{z}{1-z^2} \left(\frac{1+z}{1-z}\right)^y \exp\left(\frac{2xz^2}{1-z^2}\right) \tag{3.34}$$

where C is a constant. We then look for a solution of the full equation (3.33), of the form (3.34), where $C(z)$ is now an unknown function. We thus get

$$\frac{dC}{dz} = \frac{1}{1-z^2}\left(\frac{1+z}{1-z}\right)^{-y} \exp\left(-\frac{2xz^2}{1-z^2}\right)[d_2 - z^2 - 2y(d_1+z)] \quad (3.35)$$

The function $C(z)$ is obtained by integrating this last equation. The definition of $C(z)$ implies $C(0) = d_1$, since $f(z) \approx C(0)z$ for $z \to 0$. On the other hand, the decay of the moments d_m for large m implies $C(\pm 1) = 0$. Indeed, otherwise the generating function $f(z)$ would be exponentially divergent as $z \to \pm 1$. These three conditions determine the moments d_1 and d_2. Some algebra yields the scaling function $F(x, y)$ as the ratio of two integrals, namely

$$F(x, y) = \frac{\mathscr{J}(x, y)}{\mathscr{I}(x, y)} \quad (3.36)$$

with

$$\begin{aligned} \mathscr{I}(x, y) &= \int_{-1}^{+1} \frac{dz}{1-z^2}\left(\frac{1+z}{1-z}\right)^{y} \exp\left(-\frac{2xz^2}{1-z^2}\right) \\ \mathscr{J}(x, y) &= \int_{-1}^{+1} \frac{dz}{1-z^2}\left[x + yz + \frac{1}{2}(1-z^2)\right]\left(\frac{1+z}{1-z}\right)^{y} \exp\left(-\frac{2xz^2}{1-z^2}\right) \end{aligned} \quad (3.37)$$

It turns out that the integrals defined just above can be expressed in closed form in terms of Bessel functions, by means of the change of variable $z = \tanh(\xi/2)$, and of integrations by parts. We thus obtain

$$F(x, y) = -x\frac{d}{dx}\ln K_y(x) = \frac{x[K_{y+1}(x) + K_{y-1}(x)]}{2K_y(x)} \quad (3.38)$$

where

$$K_y(x) = \int_{-\infty}^{\infty} \frac{d\xi}{2} \exp(y\xi - x\cosh\xi) \quad (3.39)$$

is the modified Bessel function of the third kind (ref. 32, Vol. II).

The exact expression (3.38) describes the full scaling behavior of the characteristic exponent in the weak-disorder regime and close to criticality. A similar result is reported in ref. 9, although its quantitative consequences have not been explored completely.

The result (3.38) shows that $F(x, y)$ is an even function of y, implying that the characteristic exponent is symmetric in both phases $\mu > 0$ and $\mu < 0$ in the scaling region. In the following, we restrict the analysis to $\mu > 0$, i.e., $y > 0$, for definiteness. There are *a priori* six interesting limiting

situations. The case $\mu \ll \Delta^2$, to be referred to as the random critical situation, is subdivided into regime (i) ($t \ll \mu$), regime (ii) ($\mu \ll t \ll \Delta^2$), and regime (iii) ($t \gg \Delta^2$). Similarly, the case $\Delta^2 \ll \mu$, to be referred to as the weak-disorder situation, is subdivided into regime (iv) ($t \ll \Delta^2$), regime (v) ($\Delta^2 \ll t \ll \mu$), and regime (vi) ($t \gg \mu$). Some aspects of these various cases will be investigated in more detail, although we do not aim at a systematic exposition of these matters.

3.3.1. The Weak-Disorder Limit. Let us consider first the case where the strength of disorder Δ^2 goes to zero first. Both scaling variables x and y thus go to infinity simultaneously. This situation embraces regimes (v) and (vi). In this limit, the integral representation (3.39) for the Bessel function $K_y(x)$ can be estimated by the saddle-point, or steepest-descent, approximation, which can be improved via a systematic expansion around the saddle point. We thus obtain

$$K_y(x) = \left(\frac{\pi \tanh \xi_c}{2y}\right)^{1/2} \exp[y(\xi_c - \coth \xi_c)] \times \left[1 + \frac{\tanh \xi_c (5 \tanh^2 \xi_c - 3)}{24y} + \cdots\right] \tag{3.40}$$

where the saddle-point value ξ_c is such that $\sinh \xi_c = y/x$. A few more correction terms are known explicitly (ref. 32, Vol. II).

By inserting the expansion (3.40) into the result (3.38), we obtain

$$F(x, y) = (x^2 + y^2)^{1/2} + \frac{x^2}{2(x^2 + y^2)} + \frac{x^2(4y^2 - x^2)}{16(x^2 + y^2)^{5/2}} + \cdots \tag{3.41}$$

The leading term yields the expected scaling behavior $\Omega = (t^2 + \mu^2)^{1/2}$ of the characteristic exponent of the uniform chain, in the absence of disorder, implying the estimate $H(\Lambda) \approx (1/\pi)(\mu^2 - \Lambda^2)^{1/2}$ for the integrated density of states, in accord with the Bloch dispersion law $\Lambda^2 \approx q^2 + \mu^2$ [see Eqs. (2.15), (2.28)]. The correction terms in the result (3.41) are proportional to the successive powers of Δ^2. Only the last correction, proportional to Δ^4, affects the imaginary part of the scaling function, and thus the fermionic density of states.

3.3.2. The Critical Point. The behavior of the characteristic exponent at the critical point is described by the scaling function

$$F(x, 0) = \frac{xK_1(x)}{K_0(x)} \tag{3.42}$$

obtained by setting $y = 0$ in the result (3.38).

For x large, i.e., in regime (iii), the standard expansion of the Bessel function (ref. 32, Vol. II) yields

$$F(x, 0) = x + \frac{1}{2} - \frac{1}{8x} + \frac{1}{8x^2} + \cdots \tag{3.43}$$

The first two terms of this expansion match with the behavior of the result (3.23) for $\mu = 0$.

The opposite situation of x small, i.e., regime (ii), is by far more interesting, since it describes the true behavior of the characteristic exponent at the bottom of the spectrum of the random problem. We have (ref. 32, Vol. II)

$$K_0(x) = -\ln(x/2) - \gamma_E + \mathcal{O}(x^2 \ln x) \tag{3.44}$$

where $\gamma_E \approx 0.57721$ denotes Euler's constant.

The expression (3.44) yields the following logarithmic behavior for the scaling function of the characteristic exponent:

$$F(x, 0) \approx \frac{1}{\ln(2/x) - \gamma_E} \tag{3.45}$$

By inserting the continuation of the result (3.45) to $t = i\Lambda$ into Eq. (3.4), we obtain the following behavior for the integrated density of states at criticality:

$$H(\Lambda) \approx \frac{\Lambda^2}{2[\ln^2(\Lambda_0/\Lambda) + \pi^2/4]} \tag{3.46}$$

with

$$\Lambda_0 = 2e^{-\gamma_E}\Lambda^2 \approx 1.12292\Lambda^2 \tag{3.47}$$

This estimate implies the following very strong divergence for the density of states:

$$\rho(\Lambda) \approx \frac{\Lambda^2 \ln(\Lambda_0/\Lambda)}{\Lambda[\ln^2(\Lambda_0/\Lambda) + \pi^2/4]} \tag{3.48}$$

Analogous inverse logarithmic laws affect the spectra of several other one-dimensional random models at special points, e.g., harmonic chains,[33, 37] the Anderson model with nondiagonal disorder, or biased classical hopping models.[38]

It turns out that the estimates (3.46), (3.48) are still quantitatively

correct for an arbitrary distribution of the random exchange couplings, beyond the weak-disorder approximation. In that general situation, the cutoff Λ_0 is no longer given by the expression (3.47), but depends on the distribution of the random exchange couplings. This can be demonstrated by expanding Eq. (3.14) to a higher order in a_n and by checking explicitly that the higher-order terms do not alter the nature of the logarithmic behavior (3.45).

3.3.3. The Vicinity of the Critical Point. Before returning to the main subject of this article, namely the critical behavior of the ground-state energy, we have to determine first the behavior of the integrated density of states in the vicinity of the critical point, i.e., for x small and nonzero values of the scaling variable y.

The form of the scaling function $F(x, y)$ for x small and arbitrary y can be determined by means of the following formula:

$$K_y(x) = \frac{\pi}{2 \sin \pi y} [I_{-y}(x) - I_y(x)] \tag{3.49}$$

where

$$I_y(x) = \left(\frac{x}{2}\right)^y \sum_{k \geqslant 0} \frac{(x/2)^{2k}}{k!\, \Gamma(y+k+1)} \tag{3.50}$$

is the modified Bessel function of the first kind (ref. 32, Vol. II).

We thus obtain

$$F(x, y) \approx \frac{(x/2)^{-y} \Gamma(1+y) + (x/2)^y \Gamma(1-y)}{(x/2)^{-y} \Gamma(y) + (x/2)^y \Gamma(-y)} \tag{3.51}$$

In this result, which generalizes Eq. (3.45), each of the four terms is accompanied by a series of subleading powers of x^2, in virtue of the expansion (3.50).

The behavior of the density of states near the bottom of the spectrum slightly off criticality is obtained by expanding Eq. (3.51) for $x \to 0$, namely

$$F(x, y) = y + \frac{2\pi}{\Gamma^2(y) \sin \pi y} \left(\frac{x}{2}\right)^{2y} + \cdots \tag{3.52}$$

We notice that the value $F(0, y) = y$ for $x = 0$ and $y > 0$ is in accord with the general result (3.8).

By taking the imaginary part of the expression (3.52), we obtain

$$H \approx \frac{2\Delta^2}{\Gamma^2(y)} \left(\frac{\Lambda}{2\Delta^2}\right)^{2y} \tag{3.53}$$

This last estimate holds true for $|x| \ll y$, i.e., $\Lambda \ll \mu$. This range encompasses regimes (i), (iv), and (v).

Equation (3.53) implies that the density of states assumes the following scaling form for large values of y, which describes the tail of the spectrum induced in the region $\Lambda \ll \mu$ by a small amount of disorder:

$$H \sim \exp\left(-\frac{2\mu}{\Delta^2} \ln \frac{2\mu}{e\Lambda}\right) \tag{3.54}$$

This exponential falloff is reminiscent of Lifshitz tails[39] which are present near generic band edges in the spectra of disordered systems, although the present situation is different from the usual case of, e.g., the Anderson model with diagonal disorder.

It is also worth noticing that the result (3.53) implies in particular that the fermionic spectrum of the random chain extends down to $\Lambda = 0$ off criticality, whereas there is a finite gap, given by Eq. (2.29), in situations where the modulation is bounded.

3.3.4. The Ground-State Energy. In order to evaluate the singular part of the ground-state energy of the disordered spin chain, we come back to the result (3.51), concerning the characteristic exponent in the scaling region, close to criticality ($y \to 0$). We find it convenient to set

$$\Lambda = 2\Delta^2 e^{-\theta} \tag{3.55}$$

so that we have $x = 2i \exp(-\theta)$.

After some algebra, we obtain the following expression:

$$H \approx \frac{2\Delta^2}{\Gamma^2(y) \exp(2y\theta) + \Gamma^2(-y) \exp(-2y\theta) - 2\pi/(y \tan \pi y)} \tag{3.56}$$

for the integrated density of states, which holds up to terms of relative order $\exp(-2\theta)$.

The singular part of the ground-state energy can be estimated by integrating Eq. (2.8) by parts, namely

$$\mathscr{E}_{\mathrm{sg}}(\mu) \approx \tfrac{1}{2} \int_{\theta_0}^{\infty} H(\theta)\, d\Lambda(\theta) - \{\mu = 0\} \tag{3.57}$$

where θ_0 is an inessential cutoff, and where nonsingular boundary contributions have been omitted.

A first approach to the determination of the critical singularity consists in taking the leading behavior of the result (3.56) as $y \to 0$, considering the

product $y\theta$ as a fixed quantity. The lower bound of the integral in Eq. (3.57) can then be put equal to zero. We thus obtain

$$\mathscr{E}_{\mathrm{sg}} \approx -\frac{\Delta^4}{2}\mathscr{F}(y) \tag{3.58}$$

with

$$\mathscr{F}(y) = \int_0^\infty e^{-\theta}\, d\theta \left(\frac{1}{\theta^2} - \frac{y^2}{\sinh^2 y\theta}\right) \tag{3.59}$$

The scaling function $\mathscr{F}$ is clearly an even function of y. It can be brought, by means of two integrations by parts, to the following form[36, 40]:

$$\begin{aligned}\mathscr{F}(y) &= \int_0^\infty e^{-\theta}\, d\theta \ln \frac{\sinh y\theta}{y\theta} = \sum_{m \geqslant 1} \frac{B_{2m}}{2m}(2y)^{2m} \\ &= -\Psi\left(\frac{1}{2y}\right) - y - \ln(2y)\end{aligned} \tag{3.60}$$

where $\Psi(z)$ is the logarithmic derivative of Euler's function $\Gamma(z)$, and the B_n are the Bernoulli numbers (ref. 32, Vol. I).

A similar result has been established[9, 10] in the case of the two-dimensional classical Ising model. As a matter of fact, the estimate (3.58) is wrong by a constant prefactor in the weak-disorder regime, as will become clear in a while.

The function $\mathscr{F}$, and functions with a similar analytic structure, are ubiquitous in the expressions of the scaling laws describing the spectra of random systems close to band edges.[36, 40]

The result (3.58) shows that the ground-state energy is infinitely differentiable, but nonanalytic at the critical point ($y = 0$). Indeed, the Bernoulli numbers exhibit the following asymptotic growth:

$$B_{2m} \approx \frac{(-1)^{m-1}\, 2(2m)!}{(2\pi)^{2m}} \tag{3.61}$$

As a consequence, the series representation (3.60) is divergent, and only determines the function $\mathscr{F}$ up to exponentially small terms in $1/y$. These ambiguous parts could be used as a vague definition of the "singular part" of the ground-state energy.

It turns out that the result (3.58) provides a quantitative meaning to the notion of critical singularity, by means of an analytic continuation in the complex y plane. We recall that $\mathscr{F}(y)$ is an even function. Assume that

we perform its analytic continuation from $y>0$ to the whole half-plane $\mathrm{Re}\, y>0$, and from $y<0$ to the whole half-plane $\mathrm{Re}\, y<0$. Both continuations do not match along the imaginary axis. More precisely, the discontinuity between both of them at the point $y=i\,|y|$ can be evaluated by means of the difference formula for the Ψ function. We thus obtain the exact expression

$$\mathscr{F}(i\,|y|+0)-\mathscr{F}(i\,|y|-0)=\frac{2\pi i}{e^{\pi/|y|}-1} \tag{3.62}$$

We define the singular part of the ground-state energy as

$$\delta\mathscr{E}(\mu)\equiv\mathscr{E}_{\mathrm{sg}}(i\,|\mu|+0)-\mathscr{E}_{\mathrm{sg}}(i\,|\mu|-0)\approx -i\pi\Delta^4\exp\left(-\frac{\pi\Delta^2}{|\mu|}\right) \tag{3.63}$$

As we have already mentioned briefly, the estimate (3.63) misses a constant prefactor. Indeed, a more accurate expansion of the expression (3.56) for H, including terms of relative order y^2, considering still the product $y\theta$ as fixed, leads to the following formula:

$$\mathscr{E}_{\mathrm{sg}}\approx\frac{\Delta^4 y^2}{2}\int_{\theta_0}^{\infty}\frac{e^{-\theta}\,d\theta}{\sinh^2 y\theta-\gamma_{\mathrm{E}}\,y\sinh 2y\theta+(\pi^2/4+\gamma_{\mathrm{E}}^2)\,y^2} \tag{3.64}$$

The singular part $\delta\mathscr{E}(\mu)$, which we define as the discontinuity used in Eq. (3.63), can be expressed from Eq. (3.64) as a contour integral which encircles once in the counterclockwise direction the poles of the integrand with $\mathrm{Re}\,\theta>0$. The quantity $\delta\mathscr{E}(\mu)$ thus defined is independent of the cutoff θ_0. The poles come in close pairs situated at $\theta\approx n\pi/|y|$ $(n\geqslant 1)$, where $\sinh y\theta=i\sin(|y|\theta)$ is very close to zero. The leading contribution to $\delta\mathscr{E}(\mu)$ comes from the nearest pair of poles $(n=1)$, which lie at $\theta=\pi/|y|+\gamma_{\mathrm{E}}\pm i\pi/2$. Residue calculus yields

$$\delta\mathscr{E}(\mu)\approx -2i\Delta^4\exp(-\gamma_{\mathrm{E}})\exp\left(-\frac{\pi\Delta^2}{|\mu|}\right) \tag{3.65}$$

The standard analysis which led to Eqs. (3.58) and (3.63) along the lines of refs. 9 and 10 thus misses a prefactor of $(2/\pi)\exp(-\gamma_{\mathrm{E}})\approx 0.35743$, which is generated by an unexpected finite shift of the pole positions. A similar phenomenon had been underlined in ref. 12, in the framework of exactly solvable classical random Ising models.

4. APERIODIC CHAINS, THE CASE OF A BOUNDED FLUCTUATION

After having studied in detail both extreme situations of periodic and random chains, we now consider the general case, where the reduced exchange constants $\{\varepsilon_n\}$ form an arbitrary aperiodic sequence, with physically reasonable homogeneity properties, so that at least the fermionic density of states (2.9) exists.

4.1. General Results

In order to study this problem, it is natural to look at *periodic approximants*, obtained by truncating the sequence of the $\{\varepsilon_n\}$ to the first M ones and repeating this finite motif, as a unit cell, in a periodic way. The properties of the full aperiodic system are then recovered in the $M \to \infty$ limit.

We already know from Section 2.3 that the transverse-field Ising chain has a unique critical point, defined by the condition $\mu = 0$, where μ is defined in Eq. (1.4), for any sequence of exchange couplings $\{J_n\}$. The main goal of the rest of this paper is to study the form of the critical singularity of the ground-state energy in the critical region, i.e., for $\mu \to 0$. The starting point of our investigation is the outcome of Section 2.3 concerning periodic chains, and especially the expression (2.27) for the velocity v of the fermionic excitations at criticality.

It has become clear from our generalized Harris criterion, exposed in the Introduction, that the key concept is that of the *fluctuation* of the exchange couplings. Consider indeed again the partial sums g_n defined in Eq. (1.7). The sequence of reduced exchange couplings $\{\delta_n\}$ will be said to have *a bounded fluctuation* if the g_n are bounded for any number n of couplings. If this holds true, it is easily realized that the velocities v_M of the fermionic excitations on the periodic approximants with M bonds are bounded away from zero and from infinity. Under reasonable assumptions, the v_M will admit a finite limit v as $M \to \infty$.

The following two main situations are thus to be considered:

1. The velocities v_M of the periodic approximants have *a finite limit* v as $M \to \infty$. This situation is usually met for exchange couplings with *a bounded fluctuation*, in the sense defined above. Typical examples of this situation, to be treated below, include quasiperiodic chains, the Thue–Morse chain, and the random dimer model. The Ising chain then belongs to the Onsager universality class of the uniform spin chain, with an energy gap linear in $|\mu|$, according to Eq. (2.29), and a logarithmic critical singularity of the ground-state energy given by Eq. (2.33). In other words,

a modulation of the couplings with a bounded fluctuation is not sufficient to alter the critical behavior of the uniform chain.

2. The velocities v_M of the periodic approximants *diverge* as $M \to \infty$. This second situation is generically met for exchange couplings with *an unbounded fluctuation.* Typical examples of this situation include random chains, and deterministic chains generated by non-Pisot inflation rules, to be treated below. This case corresponds formally to $v = 0$, so that the critical singularity of the ground-state energy is of a weaker type than that of the uniform Ising model.

4.2. Examples of Systems with a Bounded Fluctuation

4.2.1. Quasiperiodic Chains. An important class of aperiodic sequences with a bounded fluctuation is provided by quasiperiodic sequences. Consider the exchange couplings given by the formula

$$\delta_n = f(n\omega) \tag{4.1}$$

where f is a periodic function of one variable, with unit period, and ω an irrational modulation wavenumber, or incommensurability ratio.

The sequence $\{\delta_n\}$ so defined is quasiperiodic. Indeed, its Fourier transform consists of delta functions situated at values of the wavevector of the form $q = 2\pi(k + l\omega)$, where k and l are two integers.

In most cases, the sequence defined in Eq. (4.1) has a bounded fluctuation. More precisely, we have

$$g_n = g(n\omega) \tag{4.2}$$

where the function g, called the "hull function" of the sequence,[14] is also periodic, with unit period. Moreover, the functions f and g are related through the identity

$$f(\theta) = g(\theta) - g(\theta - \omega) \tag{4.3}$$

as a consequence of Eq. (1.7).

Let us now evaluate the velocity v by means of its expression (2.27). We have

$$\varepsilon_{m+1}^2 \cdots \varepsilon_{m+k}^2 = \exp[2g(m\omega + k\omega) - 2g(m\omega)]$$

Using the equidistribution of $\{m\omega\}$ modulo unity, we can show that there exists a limit velocity as $M \to \infty$, given by the following integral formula:

$$\frac{1}{v^2} = \int_0^1 e^{2g(\theta)}\, d\theta \cdot \int_0^1 e^{-2g(\theta)}\, d\theta \tag{4.4}$$

This result provides a quantitative prediction concerning the critical singularity of an arbitrary quasiperiodic Ising chain with two incommensurate periods. It can be easily generalized to sequences with N incommensurate periods, by replacing in Eq. (4.4) the θ integrals by integrals over the $(N-1)$-torus.

Let us now consider in more detail a few examples of physical interest.

Example 1. The Quasicrystalline Chain. The most popular way of generating quasiperiodic tilings which model quasicrystalline structures consists in the so-called cut-and-projection method.[41] One-dimensional quasiperiodic binary sequences can be generated within this framework by drawing a straight line with slope $t = \tan\phi$ and projecting onto it all the lattice points of the "strip" $0 \leqslant y - tx < t + 1$, with integer coordinates.

To this geometrical construction corresponds the following discontinuous f function:

$$f(\theta) = \begin{cases} (1-\omega)\Delta & \text{for } 0 \leqslant \theta < \omega \pmod 1 \\ -\omega\Delta & \text{for } \omega \leqslant \theta < 1 \pmod 1 \end{cases} \tag{4.5}$$

with $\omega = t/(t+1)$, and where Δ is the strength of the modulation, so that $\exp(\Delta)$ is the ratio between both values assumed by the ε_n. The associated hull function reads

$$g(\theta) = \Delta\theta \qquad (0 \leqslant \theta < 1) \tag{4.6}$$

Hence the general result (4.4) yields

$$v = \frac{\Delta}{\sinh \Delta} \tag{4.7}$$

This result is independent of the incommensurability ratio ω, provided the latter is an irrational number. It had been established[19, 20] in the particular case of the Fibonacci chain, corresponding to $\omega = 1/\tau^2$, where $\tau = (1+\sqrt{5})/2$ is the golden mean. For rational values of ω, periodic chains are generated. For $\omega = 1/2$, the result (2.34) is recovered, whereas, e.g., for $\omega = 1/3$ and $\omega = 2/3$ we obtain

$$v = \frac{3}{1 + 2\cosh(2\Delta/3)} \tag{4.8}$$

Example 2. The Harmonic Incommensurate Chain. Our second example of a quasiperiodic chain is defined by the following harmonic modulation:

$$f(\theta) = \frac{\Delta}{2}\cos 2\pi\theta \tag{4.9}$$

The associated hull function reads

$$g(\theta)=\frac{\Delta}{4}\frac{\sin(2\pi\theta+\pi\omega)}{\sin\pi\omega} \tag{4.10}$$

so that we obtain

$$\frac{1}{v}=I_0\left(\frac{\Delta}{2\sin\pi\omega}\right) \tag{4.11}$$

where I_0 denotes the modified Bessel function of the first kind and order zero (ref. 32, Vol. II).

In the present case, the velocity of fermionic excitations depends on the incommensurability ratio ω. In the regime of a long modulation wavelength $\lambda=1/\omega\gg 1$, this velocity vanishes exponentially as

$$v\sim\exp\left(-\frac{\lambda\Delta}{2\pi}\right) \tag{4.12}$$

(Counter-)Example 3. Circle-Map Sequences. We end up this section by describing a class of binary sequences which generically exhibit a weakly unbounded modulation in spite of their quasiperiodic nature. These mathematical objects are defined by a circle map,[16, 17] which is a generalization of the cut-and-project model, obtained by allowing the discontinuity point ζ of the f function of Eq. (4.5) to be different from the modulation wavevector ω, namely

$$f(\theta)=\begin{cases}(1-\zeta)\Delta & \text{for } 0\leqslant\theta<\zeta \pmod 1\\ -\zeta\Delta & \text{for } \zeta\leqslant\theta<1 \pmod 1\end{cases} \tag{4.13}$$

It has been shown[15] that the circle-map sequence $\{\delta_n=f(n\omega)\}$ possesses a hull function and a bounded fluctuation if, and only if, the parameters ω and ζ obey the following "Kesten condition"[42]:

$$\zeta=r\omega \pmod 1 \tag{4.14}$$

for some (positive or negative) integer r. In particular, the cut-and-project algorithm, exposed in Example 1 above, is recovered for $r=1$.

Whenever the Kesten condition (4.14) holds, the hull function $g(\theta)$ can be written explicitly.[16] This outcome yields the following expression, assuming $r\geqslant 1$ for definiteness:

$$\frac{1}{v^2}=\frac{1}{4r^2\Delta^2}\sum_{k=1}^{r}e^{2\Delta k}(e^{-2r\Delta\theta_{k-1}}-e^{-2r\Delta\theta_k})$$
$$\times\sum_{l=1}^{r}e^{-2\Delta l}(e^{2r\Delta\theta_l}-e^{-2r\Delta\theta_{l-1}}) \tag{4.15}$$

with $\theta_0 = 0 < \theta_1 < \cdots < \theta_{r-1} < \theta_r = 1$, and $\{\theta_1, ..., \theta_{r-1}\}$ is the ordered sequence of the numbers $m\omega$ (mod 1), for $m = 1, ..., r-1$.

For generic values of (ω, ζ), which do not fulfill the Kesten condition (4.14), the circle-map sequence has an unbounded fluctuation, even though it is a quasiperiodic sequence. The law of divergence of the partial sums g_n depends in a complicated fashion on Diophantine properties of both parameters (see, e.g., ref. 43). The typical case is that of a logarithmic divergence of the fluctuation,[15] which is sufficient for the velocity v to vanish, and thus for the Onsager singularity to be altered. We will show in Section 5.2 that this situation corresponds to a continuously varying negative specific heat exponent α.

4.2.2. The Random Dimer Model. The random dimer chain is an interesting example of a random sequence $\{\delta_n\}$, so that the associated fluctuation g_n is bounded. Hence the model, although it is disordered, belongs to the Onsager universality class.

The model is defined as a random mixture of "dimers," i.e., binary molecules, which are either AB or BA, chosen independently with respective probabilities p and $(1-p)$. We attribute to the letters two different exchange couplings, namely $\delta_A = \Delta/2$ and $\delta_B = -\Delta/2$. In other words, we have, independently for every k,

$$\begin{aligned} &\{\delta_{2k-1} = \Delta/2, \quad \delta_{2k} = -\Delta/2\} \qquad \text{with prob. } p \\ &\{\delta_{2k-1} = -\Delta/2, \quad \delta_{2k} = \Delta/2\} \qquad \text{with prob. } 1-p \end{aligned} \tag{4.16}$$

This definition ensures that the fluctuation is bounded, since it can assume only three values, namely $g_n = 0, \pm\Delta/2$.

The evaluation of the velocity v goes as follows. First, we have the identity $\varepsilon_{2k-1}\varepsilon_{2k} = 1$, so that only the products of one or two consecutive couplings ε_n remain in the expression (2.27). Second, we have, in the sense of averaging over disorder,

$$\overline{\varepsilon_{2k}^2} = (1-p)e^{\Delta} + pe^{-\Delta}, \qquad \overline{\varepsilon_{2k+1}^2} = pe^{\Delta} + (1-p)e^{-\Delta} \tag{4.17}$$

and hence, in the sense of Cesàro averages, as introduced in Eq. (1.4),

$$\begin{aligned} \overline{\varepsilon_n^2} &= \tfrac{1}{2}(\overline{\varepsilon_{2k-1}^2} + \overline{\varepsilon_{2k}^2}) = \cosh \Delta \\ \overline{\varepsilon_n^2 \varepsilon_{n+1}^2} &= \tfrac{1}{2}(1 + \overline{\varepsilon_{2k}^2}\,\overline{\varepsilon_{2k+1}^2}) = 1 + 2p(1-p)\sinh^2 \Delta \end{aligned} \tag{4.18}$$

We thus obtain

$$1/v^2 = \cosh^2(\Delta/2)[1 + 4p(1-p)\sinh^2(\Delta/2)] \tag{4.19}$$

For $p=0$ or $p=1$, the dimer chain is a periodic binary chain, and the result (2.34) is recovered. In the most random situation of the symmetric dimer chain ($p=1/2$), the velocity assumes its minimal value, namely

$$v=\frac{1}{\cosh^2(\Delta/2)} \tag{4.20}$$

4.2.3. The Thue–Morse Chain. The Thue–Morse sequence is a simple example of an aperiodic deterministic sequence which is self-similar, owing to its recursive construction by iteration of a substitution, i.e., inflation rules. Some general formalism about substitutions will be presented in Section 5.1.

For the time being, we consider the sequence defined by the following substitution:

$$\sigma: \begin{cases} A \to AB \\ B \to BA \end{cases} \tag{4.21}$$

By the repeated action of these rules, starting with the letter A, we generate an infinite binary sequence, $\Sigma = ABBABAABBAABABBA\ldots$, known as the Thue–Morse sequence, which has remarkable arithmetical properties. The reader interested in a more mathematically oriented background is referred to ref. 44.

A numerical sequence of exchange couplings is defined by taking the value $\delta_n=\Delta/2$ if the nth letter in Σ is an A, and the value $\delta_n=-\Delta/2$ if the nth letter in Σ is a B. The sequence so defined is nothing but a particular configuration of the random dimer chain considered in Section 4.2.2. It has therefore a bounded fluctuation. The Thue–Morse sequence is nevertheless neither periodic nor quasiperiodic. As a matter of fact, its diffraction spectrum (Fourier transform) does not contain any Bragg peak; it is known to be a purely singular continuous measure.[44]

It can be shown, along the very lines of the previous example, that the velocity v for the Thue–Morse sequence coincides with that of the symmetric random dimer chain, namely

$$v=\frac{1}{\cosh^2(\Delta/2)} \tag{4.22}$$

This result has already been obtained in ref. 27.

Surprisingly enough, it turns out that the periodic sequence with motif $ABBA$, the symmetric ($p=1/2$) random dimer sequence, and the aperiodic deterministic Thue–Morse sequence all have the same value for the velocity v of fermionic excitations. This quantity is therefore fully insensitive to the "type of order" of the structure, and especially to its Fourier spectrum.

5. APERIODIC CHAINS. THE CASE OF AN UNBOUNDED FLUCTUATION

5.1. The Generic Case: Power-Law Fluctuation

We have shown in the beginning of Section 4 that the critical singularity of the Ising chain in a transverse field is weaker than the Onsager singularity whenever the sequence of exchange couplings has an unbounded fluctuation in the sense defined in the Introduction. This result confirms the generalized Harris criterion exposed there.

The case of independent random exchange couplings has been studied in Section 3. We have shown that the critical singularity is of an essential type, namely that all the derivatives of the ground-state energy w.r.t. the temperaturelike variable μ are finite at the critical point $\mu = 0$. We now investigate the case of an arbitrary sequence of exchange couplings with an unbounded fluctuation. Examples of such sequences of physical interest are provided by binary self-similar sequences, generated by non-Pisot substitutions, a concept to be defined later.

Some general formalism about substitutions will be needed. Let us take, for definiteness, the example of the following substitution rules, which have been described in refs. 45 and 46, in connection with nonquasiperiodic binary tilings of the plane with fivefold symmetry:

$$\sigma: \begin{vmatrix} A \to AAAB \\ B \to BBA \end{vmatrix} \tag{5.1}$$

We consider the words $A_k = \sigma^k(A)$ and $B_k = \sigma^k(B)$ obtained by the repeated action of the substitution rules on the initial letters. Since $\sigma(A)$ begins with A, the A_k converge to an infinite sequence Σ, which is left invariant by the substitution σ, and hence self-similar.

To the above rules is attached the substitution matrix

$$\mathbf{M} = \begin{pmatrix} \text{number of } A\text{'s in } \sigma(A) & \text{number of } A\text{'s in } \sigma(B) \\ \text{number of } B\text{'s in } \sigma(A) & \text{number of } B\text{'s in } \sigma(B) \end{pmatrix} = \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix} \tag{5.2}$$

The eigenvalues and eigenvectors of the matrix $\mathbf{M}$ govern most geometrical characteristics of the sequence Σ. The densities (ρ_A, ρ_B) of both letter types are given by the normalized right eigenvector associated with the eigenvalue λ_1 with largest modulus, which is real and positive, in virtue of the Perron–Frobenius theorem.

The sequence of exchange couplings at criticality is obtained by setting $\delta_n = \delta_A = \rho_B \Delta$ (respectively, $\delta_n = \delta_B = -\rho_A \Delta$) if the nth letter in the

sequence Σ is an A (respectively, a B), where $\Delta > 0$ denotes the strength of the aperiodic modulation.

We are led to wonder whether a sequence generated by substitution rules has a bounded fluctuation or not. The answer is simple. The demarcation line lies between *Pisot* and *non-Pisot* substitutions. The same criterion plays a central role in the study of the diffraction spectra (i.e., Fourier transforms) of self-similar chains and tilings.[45, 47–49]

1. A substitution is said to have the Pisot–Vijayaraghavan property, or Pisot property for short,[45, 48] if the second largest eigenvalue λ_2 of the associated matrix is smaller than unity in modulus. This terminology originates in the closely related concept of Pisot algebraic numbers.[50, 51] The sequences generated by Pisot substitutions have a bounded fluctuation, and usually a discrete diffraction spectrum (Fourier transform). They provide examples of self-similar quasiperiodic—or almost periodic—structures.

2. A substitution such that $|\lambda_2| \geqslant 1$ is said to be non-Pisot. A non-Pisot substitution generates sequences for which the fluctuation g_n defined in Eq. (1.7) diverges as a power law. This can be understood as follows. The length of the word A_k, i.e., the number of its letters, scales as λ_1^k. The associated fluctuation of the exchange couplings, i.e., the sum $g(A_k)$ of the δ_n associated with the word A_k, does not scale as λ_1^k, but only as $|\lambda_2|^k$. Indeed, otherwise the model would not be at criticality. Eliminating the generation label k between both above estimates, we obtain the power law $g_n \sim n^\beta$, where the "wandering exponent" β reads

$$\beta = \frac{\ln |\lambda_2|}{\ln \lambda_1} \tag{5.3}$$

A more accurate result has been shown in a rigorous way,[52] namely

$$g_n \approx n^\beta F\left(\frac{\ln n}{\ln \lambda_1}\right) \tag{5.4}$$

where the amplitude F is a "fractal function," which is periodic in its argument, with period unity, and continuous, but nowhere differentiable.

In the case of the above example, the substitution matrix $\mathbf{M}$ has been given in Eq. (5.2). Its eigenvalues are $\lambda_1 = 2 + \tau = 3.61803$ and $\lambda_2 = 3 - \tau = 1.38197$, where $\tau = (1 + \sqrt{5})/2$ denotes the golden mean. We have $\rho_A = \tau - 1 = 1/\tau$ and $\rho_B = 2 - \tau = 1/\tau^2$. The substitution is non-Pisot, with a wandering exponent $\beta = 0.25157$.

The self-similar sequence $\{\delta_n\}$ describing the couplings at criticality possesses highly nontrivial correlations, so that the explicit scaling analysis

of Section 3 cannot be made in the present case. We have nevertheless developed a heuristic scaling approach, according to which the critical singularity is of an essential type, which is determined by the wandering exponent β.

The argument uses the formalism of the complex characteristic exponent introduced in Section 3. It goes as follows. Consider a large periodic approximant to the structure, with $M \gg 1$ exchange couplings per unit cell. A natural choice consists in taking a word A_k for such a unit cell. The result (2.27) implies that typical values of the velocity v are of order

$$v_{\text{typ}} \sim \exp(-a\, \Delta M^{\beta}) \tag{5.5}$$

for some constant a, which may depend on the more quantitative meaning that is given to the above estimate, like, e.g., the average of v taken over all the words with length M present in the sequence. Such an accuracy is not needed in the present argument.

We expect that the wavefunctions of the first low-lying fermionic excitations (with $\Delta \ll 1$) are very similar in the aperiodic structure and in its large approximants ($M \gg 1$), at least for a weak modulation of the exchange couplings ($\Delta \ll 1$). As a consequence, we can infer from the initial dispersion relation $\Delta \approx vq$ of the approximants that a scaling law of the form $\Delta \sim v_{\text{typ}} q$ holds for both q and H of order a few times $1/M$. We thus obtain

$$H \sim \left(\frac{\Delta}{|\ln \Delta|} \right)^{1/\beta} \tag{5.6}$$

and, using Eq. (3.4),

$$\Omega \sim \frac{\Delta^{1/\beta}}{|\ln t|^{(1-\beta)/\beta}} \tag{5.7}$$

The critical singularity of the ground-state energy can then be evaluated as follows. The singular part $\mathscr{E}_{\text{sg}}(\mu)$ is generated by the contribution to the integral (2.8) of the lowest values of the fermionic excitation energies Δ over a range $\delta\Delta$ which can be estimated by equating the result (5.7) for $\mu = 0$ and $t \neq 0$ with the exact expression (3.8) for $\mu \neq 0$ and $t = 0$. We thus obtain

$$\mathscr{E}_{\text{sg}}(\mu) \sim \exp[-C(\Delta\, |\mu|^{-\beta})^{1/(1-\beta)}] \tag{5.8}$$

The scaling results (5.6)–(5.8) are the main outcome of this section. They are supposed to give the correct dependence in the variables Δ, t, and μ, respectively. The dependence on Δ holds *a priori* for $\Delta \ll 1$. We have thus

shown that the ground-state energy has an exponentially small essential critical singularity, as soon as the wandering exponent β is not zero.

It is remarkable that the results (5.6)–(5.8) coincide with the outcomes of the exact scaling analysis of Section 3 in the case of independent random couplings, which corresponds to $\beta = 1/2$ [see, respectively, Eqs. (3.46), (3.45), and (3.65)].

We have verified the above general results by means of numerical work in the case of deterministic aperiodic sequences generated by substitutions. We have considered the following three examples of non-Pisot sequences:

Example 1. The sequence generated by the substitution defined in Eq. (5.1). This example corresponds to the value $\beta = 0.25157$ of the wandering exponent.

Example 2. The Rudin–Shapiro sequence. Besides its arithmetical properties,[44] this sequence can be defined by the following substitution rules, acting on four letters:

$$\sigma: \begin{vmatrix} A \to AC \\ B \to DC \\ C \to AB \\ D \to DB \end{vmatrix} \tag{5.9}$$

A binary sequence is obtained by associating the value $\delta_n = \Delta/2$ to the letters A and C, and the value $\delta_n = -\Delta/2$ to the letters B and D. The Rudin–Shapiro sequence has the remarkable property that the intensity $S(q) = 1$ of its Fourier transform coincides with the white-noise spectrum of a sequence of independent random variables. In other words, the sequence has no nontrivial two-point correlations, and a wandering exponent $\beta = 1/2$. This last property is in accord with the general result (5.3), since the eigenvalues of the 4×4 Rudin–Shapiro substitution matrix are 2, $\pm\sqrt{2}$, and 0.

Example 3. The substitution

$$\sigma: \begin{vmatrix} A \to ABBB \\ B \to AAA \end{vmatrix} \tag{5.10}$$

is one of the simplest cases with a "large" wandering exponent $\beta > 1/2$. Indeed, the eigenvalues $\lambda_1 = (1 + \sqrt{37})/2 = 3.54138$, and $\lambda_2 = (1 - \sqrt{37})/2 = -2.54138$ yield $\beta = 0.73760$.

For each of the above three examples, we have evaluated numerically the characteristic exponent Ω out of the spectrum for small real values of t. To do so, we have used the recursion relation (3.2) to generate a long

sequence of 10^5–10^6 Riccati variables for every value of t, starting, e.g., with $R_0 = \infty$, and evaluated Ω according to the formula (3.3).

Figure 1 shows plots of $\Omega^{\beta/(1-\beta)}$ against $|\ln t|$ for two moderate strengths Δ of the aperiodic modulation in each case. The very good least-square fits, shown as dashed lines, confirm the t dependence of the prediction (5.7). Oscillations around the mean power-law behavior are also clearly visible. They reflect the self-similarity of the underlying structure under a discrete dilatation group generated by the scaling factor λ_1.

More surprisingly, the Δ dependence of the characteristic exponent is found in very good agreement with the small-Δ power-law estimate (5.7), even though the values of the strength of the modulation Δ are of order unity. In order to illustrate this, we have extracted effective exponents β_{eff} from the ratio of both fitted slopes shown on Fig. 1, for each example, assuming that Ω is exactly proportional to $\Delta^{1/\beta}$. We thus get the following striking agreement:

$$\begin{aligned} &\text{Example 1:} \quad \beta_{\text{eff}} \approx 0.24, \quad \beta = 0.25157 \\ &\text{Example 2:} \quad \beta_{\text{eff}} \approx 0.50, \quad \beta = 1/2 \\ &\text{Example 3:} \quad \beta_{\text{eff}} \approx 0.74, \quad \beta = 0.73760 \end{aligned} \tag{5.11}$$

5.2. The Marginal Case: Logarithmic Fluctuation

We now investigate the case of the marginal non-Pisot substitutions, with a vanishing wandering exponent. For binary sequences, this occurs when the second eigenvalue of the substitution matrix reads $\lambda_2 = \pm 1$. Examples of such sequences with physical interest have been discussed in refs. 15–17.

We choose to consider two specific examples, for the sake of simplicity.

Example 1. The period-doubling sequence describes the symbolic dynamics of the critical trajectory of a map of the interval at the accumulation point of the period-doubling cascade (see, e.g., ref. 53). This sequence can be alternatively defined by the substitution rules

$$\sigma: \begin{vmatrix} A \to AB \\ B \to AA \end{vmatrix} \tag{5.12}$$

The eigenvalues of the associated matrix are $\lambda_1 = 2$ and $\lambda_2 = -1$.

Example 2. The circle-map sequence is a particular case of the quasiperiodic sequence defined in Eq. (4.13), corresponding to the values $\omega = 1/\tau^2$, where $\tau = (1+\sqrt{5})/2$ again denotes the golden mean, and

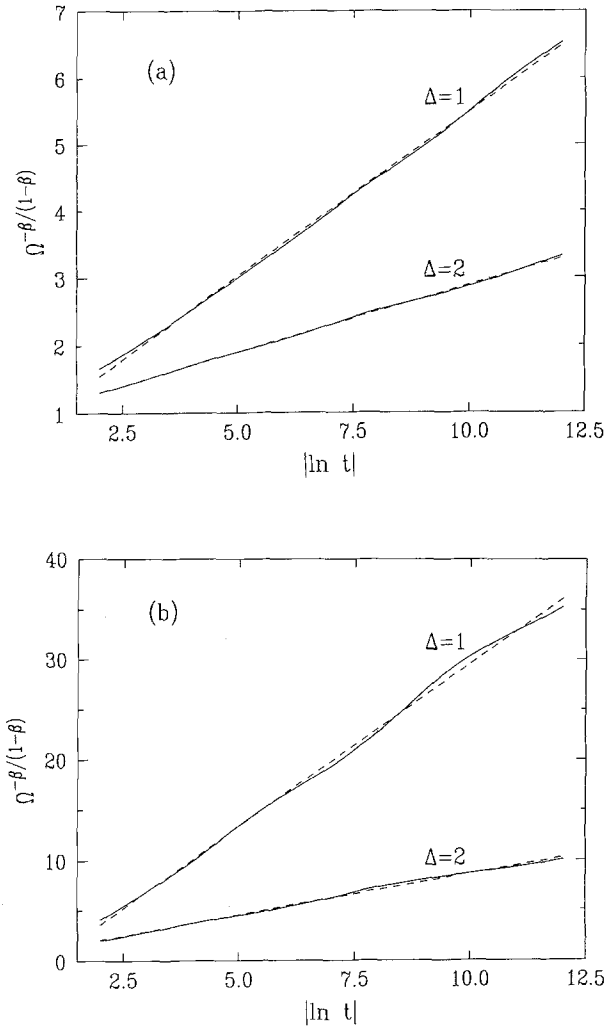

Fig. 1. Plot of numerical values of the quantity $\Omega^{-\beta/(1-\beta)}$, against $|\ln t|$, where $t>0$ is the spectral variable out of the fermionic spectrum and $\Omega(t)$ is the characteristic exponent. The straight dashed lines show least-square fits, demonstrating the t dependence of the scaling law (5.7). Two values of the modulation strength Δ, indicated on the curves, are considered in each of the following examples. (a) Example 1 [see Eq. (5.1)]. (b) Example 2 [the Rudin–Shapiro sequence) [see Eq. (5.9)]. (c) Example 3 [see Eq. (5.10)]. The ratio of both slopes in each example allows one to confirm the Δ dependence of the scaling law (5.7) [see text and Eq. (5.11)].

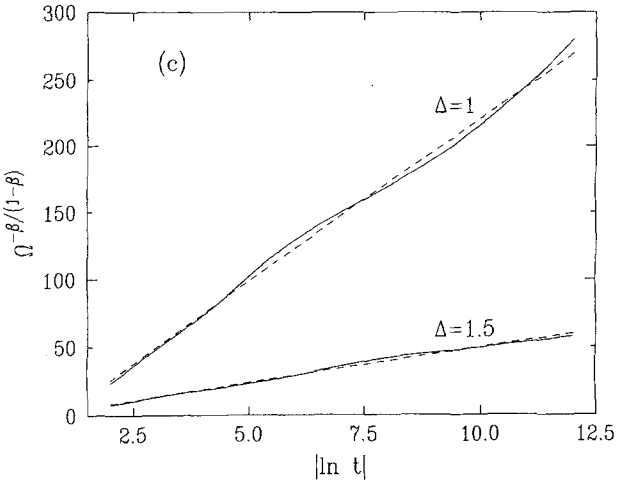

Fig. 1. (*Continued*)

$\zeta = 1/2$. These values do not fulfill the Kesten condition (4.14), so that the associated fluctuation is unbounded. It has been shown[17] that the sequence corresponding to the above values of parameters is self-similar and can be generated by the following substitution rules, acting on three letters:

$$\sigma: \begin{cases} A \to CAC \\ B \to ACCAC \\ C \to ABCAC \end{cases} \tag{5.13}$$

The eigenvalues of the associated matrix read $\lambda_1 = \tau^3$, $\lambda_2 = -1$, and $\lambda_3 = -1/\tau^3$.

In both above examples, the wandering exponent β vanishes. It has been shown[52] that the fluctuation g_n takes place on a logarithmic scale in such situations. More quantitative results, involving partial averages, read as follows:

$$\frac{1}{N}\sum_{n=1}^{N} g_n^{2p} \approx (2p-1)!!\,(w\Delta^2 \ln N)^p \tag{5.14}$$

where w is a positive constant, depending on the substitution. The similar quantities with odd exponents are subleading by at least one power of $\ln N$. These rigorous estimates suggest that the reduced variable $z_n = g_n/(\omega\Delta^2 \ln n)^{1/2}$ is asymptotically similar to a normalized Gaussian random variable.

Using this observation, we are led to assert the following power law:

$$v_{\text{typ}} \sim M^{\alpha(\Delta)} \tag{5.15}$$

along the lines of Section 5.1. Moreover, the exponent $\alpha(\Delta)$ is given by

$$\alpha(\Delta) \approx -b\Delta^2 \tag{5.16}$$

in the regime where the modulation strength Δ is small, where b is another numerical constant, characteristic of the substitution.

Following the argument of Section 5.1, we can deduce from the estimate (5.15) the power laws

$$\Omega \sim t^{1/(1-\alpha(\Delta))} \tag{5.17}$$

and finally

$$\mathscr{E}_{\text{sg}}(\mu) \sim |\mu|^{2-\alpha(\Delta)} \tag{5.18}$$

We have thus shown that the case of marginal substitutions yields, via the logarithmic scale of its fluctuation, the interesting phenomenon of the occurrence of *a negative specific heat exponent* $\alpha(\Delta) < 0$, which varies

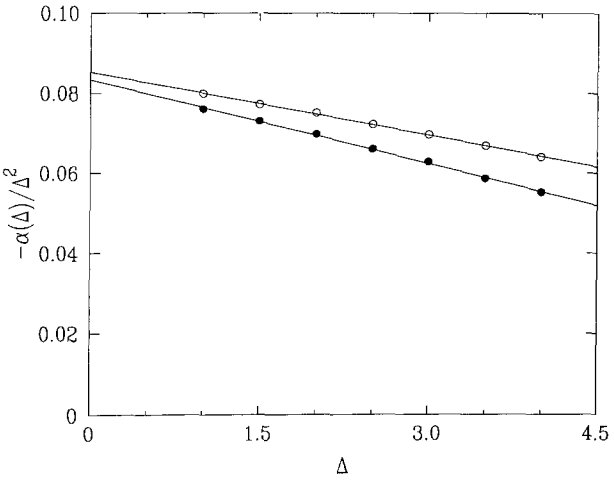

Fig. 2. Plot of the ratio $-\alpha(\Delta)/\Delta^2$ against the modulation strength Δ, where $\alpha(\Delta)$ is the negative specific heat exponent occurring in the scaling laws (5.17), (5.18) in the marginal case of a logarithmically growing fluctuation. The symbols show numerical values obtained by fitting data concerning the characteristic exponent to the power law (5.17). Two examples are considered. Open symbols: Example 1 (the period-doubling sequence) [see Eq. (5.12)]. Full symbols: Example 2 (the "circle" sequence) [see Eq. (5.13)]. The quadratic law (5.16) is clearly observed, with $b \approx 0.08$, and a small linear correction.

continuously with the strength Δ of the modulation, and vanishes quadratically for small Δ, according to Eq. (5.16).

The above predictions have been checked numerically in both examples described above. In each case, we have evaluated the characteristic exponent Ω for small real values of t, according to the procedure described in Section 5.1. The power law (5.17) is observed to a high accuracy, so that we can extract from the data very precise values for the exponent $\alpha(\Delta)$.

Figure 2 shows a plot of the ratio $-\alpha(\Delta)/\Delta^2$ against Δ. The straight lines, meant as guides for the eye, show that the quadratic law (5.16) is well verified on both examples, with a small linear correction term, up to values of order $\Delta \sim 4$. This numerical analysis yields the value $b \approx 0.08$ for both the period-doubling sequence and the circle sequence.

6. DISCUSSION

The present work shows that the interplay between geometrical characteristics of aperiodic structures and their physical properties can be understood in a thorough and quantitative fashion in one nontrivial example, namely the transverse-field ferromagnetic quantum Ising chain.

The starting point of this analysis is the formal solution of the model by means of an exact mapping onto free fermions by means of a Jordan–Wigner transformation. This has allowed us to locate exactly the critical point of the model, following previous authors,[18–31] and to identify the mechanism responsible for the critical singularity, at least in the case of the thermodynamic ground-state energy $\mathscr{E}$. The next essential feature is the simple nature of the long-distance physics which takes place in the "continuum limit," i.e., in the scaling region of the fermionic spectrum ($\mu \to 0$, $\Delta \to 0$). It is indeed remarkable that the wavefunctions admit a perturbative series expansion around the special point $\Delta = 0$, where the transfer matrices commute among themselves. This point had already been noticed to some extent in refs. 11, 19–22, 24, 27, and 30.

First, and from a qualitative viewpoint, we have generalized the Harris criterion and shown that the boundedness of the fluctuation g_n of the reduced couplings at criticality is the key concept which demarcates the "Onsager universality class" from the models with weaker critical singularities. This result can be rephrased in the language of the renormalization group. A bounded fluctuation yields a finite renormalization of the velocity v of fermionic excitations at criticality, so that only the prefactor of the logarithmic critical singularity is affected. An unbounded fluctuation is relevant; it yields an infinite renormalization of v, which vanishes as the reciprocal of either a power or an exponential of the length scale M, inducing thus a weaker type of critical singularity. These general results are

in accord with the outcomes of previous work, and especially with those of refs. 30 and 31, where it has been shown that, among the deterministic self-similar sequences generated by substitutions, only the Pisot sequences defined in Section 5 belong to the Onsager universality class.

Second, we have derived quantitative predictions concerning the critical behavior of the ground-state energy, which fully confirm our qualitative analysis, as well as the results of previous work. For chains with a bounded fluctuation (Section 4), the logarithmic singularity has an amplitude proportional to the finite velocity v of the massless fermionic excitations. In the case of quasiperiodic sequences, the prediction (4.4) holds for an arbitrary quasiperiodic modulation with one incommensurability ratio, encompassing thus many previous results as particular cases. It can be easily generalized to N incommensurate periods.

For the disordered Ising chain with independent random couplings (Section 3), we have obtained a closed-form expression (3.38) for the complex characteristic exponent in the scaling region of the weak-disorder regime. Among other outcomes, we have determined the absolute prefactor of the essential singularity of the ground-state energy—a difficult task when using other approaches.

The situation of generic sequences with an unbounded fluctuation (Section 5), with the example of non-Pisot self-similar chains, is both the most novel and the most interesting in our opinion. Indeed, previous studies of these matters[30, 31] did not provide quantitative information on the critical behavior. We have proposed a heuristic scaling argument, which is confirmed by numerical analysis to a high degree of accuracy, in the following two main cases. If the asymptotic growth of the fluctuation obeys a power law, with a wandering exponent β—this is the generic situation—there is an exponentially small essential critical singularity, depending on β, reminiscent of the case of the disordered chain. In the marginal case of a logarithmically growing fluctuation, we predict a negative specific heat exponent $\alpha(\Delta)$, which varies continuously with the strength of the aperiodic modulation.

Among possible further extensions of this work, let us mention Griffiths singularities.[54] In random classical spin models, it is known that the critical point is usually not an isolated singularity of the free energy. There is indeed a whole temperature interval, called the Griffiths phase, where thermodynamic quantities are not analytic functions of the magnetic field and/or the temperature. It has been proposed in ref. 55 to study this phenomenon by means of the fermionic representation of the two-dimensional Ising model. Griffiths singularities may also affect models with deterministic couplings which exhibit an unbounded fluctuation. On the other hand, the present work has only dealt with the ground-state energy of the quantum

spin chain. It would be desirable to extend some of the results to spin correlation functions, susceptibilities, and so on, both in the ground state and at finite temperature. A first step consists in analyzing the fermionic Green's functions. This question is essentially solved in the simpler case of the "ordinary" band edges of random systems, i.e., Lifshitz singularities.[39]

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REFERENCES

1. T. Janssen and J. Los, *Phase Transitions* **32**:29 (1991).
2. H. Hiramoto and M. Kohmoto, *Int. J. Mod. Phys. B* **6**:281 (1992).
3. J. Bellissard, A. Bovier, and J. M. Ghez, *Rev. Math. Phys.* **4**:1 (1992).
4. J. Bellissard, in *From Number Theory to Physics*, M. Waldschmidt, P. Moussa, J. M. Luck, and C. Itzykson, eds. (Springer, Berlin, 1992).
5. J. M. Luck, *Phys. Rev. B* **39**:5834 (1989).
6. E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys.* **16**:407 (1961).
7. M. Suzuki, *Phys. Lett.* **34A**:94 (1971); S. Krinsky, *Phys. Lett.* **39A**:169 (1972); E. Fradkin and L. Susskind, *Phys. Rev. D* **17**:2637 (1978).
8. L. Onsager, *Phys. Rev.* **65**:117 (1944).
9. B. M. McCoy and T. T. Wu, *Phys. Rev. Lett.* **21**:549 (1968); *Phys. Rev.* **176**:631 (1968); B. M. McCoy, *Phys. Rev. B* **2**:2795 (1970).
10. B. M. McCoy and T. T. Wu, *The 2D Ising Model* (Harvard University Press, Cambridge, Massachusetts, 1973).
11. H. Au-Yang and B. M. McCoy, *Phys. Rev. B* **10**:886 (1974).
12. Th. M. Nieuwenhuizen and H. Orland, *Phys. Rev. B* **40**:5094 (1989).
13. A. B. Harris, *J. Phys. C* 7:1671 (1974).
14. S. Aubry, *J. Phys.* (Paris) **44**:147 (1983).
15. C. Godrèche, J. M. Luck, and F. Vallet, *J. Phys. A* **20**:4483 (1987).
16. S. Aubry, C. Godrèche, and J. M. Luck, *Europhys. Lett.* **4**:639 (1987).
17. S. Aubry, C. Godrèche, and J. M. Luck, *J. Stat. Phys.* **51**:1033 (1988).
18. M. M. Doria and I. I. Satija, *Phys. Rev. Lett.* **60**:444 (1988).
19. C. A. Tracy, *J. Stat. Phys.* **51**:481 (1988).
20. H. A. Ceccatto, *Phys. Rev. Lett.* **62**:203 (1989).
21. V. Benza, *Europhys. Lett.* **8**:321 (1989).
22. F. Igloi, *J. Phys. A* **21**:L911 (1988).
23. I. I. Satija and M. M. Doria, *Phys. Rev. B* **38**:5174 (1988); **39**:9757 (1989).
24. H. A. Ceccatto, *Z. Phys. B* **75**:253 (1989).
25. M. M. Doria, F. Nori, and I. I. Satija, *Phys. Rev. B* **39**:6802 (1989).
26. Z. Lin and R. Tao, *Phys. Lett. A* **150**:11 (1990); *J. Phys. A* **25**:2483 (1992).
27. J. Q. You, X. Zeng, T. Xie, and J. R. Yan, *Phys. Rev. B* **44**:713 (1991).
28. M. Henkel and A. Patkos, *J. Phys. A* **25**:5223 (1992).
29. W. Deng, Y. Liu, D. Zheng, and C. Gong, *J. Phys. A* **25**:4757 (1992).
30. C. A. Tracy, *J. Phys. A* **21**:L603 (1988).

31. V. Benza, M. Kolar, and M. K. Ali, *Phys. Rev. B* **41**:9578 (1990).
32. A. Erdélyi, ed., *Higher Transcendental Functions*, 3 vols. (McGraw-Hill, New York, 1953).
33. Th. M. Nieuwenhuizen, *Physica* **113A**:173 (1982).
34. B. Derrida and E. Gardner, *J. Phys.* (Paris) **45**:1283 (1984).
35. Ph. Bougerol and J. Lacroix, *Products of Random Matrices, with Applications to Schrödinger Operators* (Birkhäuser, Boston, 1985).
36. J. M. Luck, *Systèmes Désordonnés Unidimensionnels* (Collection Aléa, Saclay, 1992).
37. F. Dyson, *Phys. Rev.* **92**:1331 (1953).
38. J. P. Bouchaud, A. Comtet, A. Georges, and P. Le Doussal, *Ann. Phys.* **201**:285 (1990).
39. Th. M. Nieuwenhuizen, *Physica* **167A**:43 (1990).
40. J. P. Clerc, G. Giraud, J. M. Laugier, and J. M. Luck, *Adv. Phys.* **39**:191 (1990).
41. N. G. de Bruijn, *Ned. Akad. Wet. Proc. A* **43**:39 (1981); M. Duneau and A. Katz, *Phys. Rev. Lett.* **54**:2688 (1985); *J. Phys.* (Paris) **47**:181 (1986); V. Elser, *Phys. Rev. B* **32**:4892 (1985); P. A. Kalugin, A. Yu. Kitayev, and L. S. Levitov, *J. Phys. Lett.* (Paris) **46**:L601 (1985); *JETP Lett.* **41**:145 (1985).
42. H. Kesten, *Acta Arith.* **12**:193 (1966).
43. L. Kuipers and H. Niederreiter, *Uniform Distribution of Sequences* (Wiley, New York, 1974).
44. M. Queffélec, *Substitution Dynamical Systems. Spectral Analysis* (Springer, Berlin, 1987).
45. C. Godrèche and J. M. Luck, *Phys. Rev. B* **45**:176 (1992).
46. C. Godrèche and F. Lançon, *J. Phys. I* (Paris) **2**:207 (1992).
47. E. Bombieri and J. E. Taylor, *J. Phys.* (Paris) **C3**:19 (1987); *Contemp. Math.* **64**:241 (1987).
48. C. Godrèche and J. M. Luck, *J. Phys. A* **23**:3769 (1990).
49. J. M. Luck, C. Godrèche, A. Janner, and T. Janssen, *J. Phys. A* **26** (1993).
50. C. Pisot, *Ann. Scuola Norm. Sup. Pisa* **7**:205 (1938).
51. J. W. S. Cassels, *An Introduction to Diophantine Approximation* (Cambridge University Press, Cambridge, 1957).
52. J. M. Dumont, in *Number Theory and Physics*, J. M. Luck, P. Moussa, and M. Waldschmidt, eds. (Springer, Berlin, 1990), and references quoted therein.
53. P. Collet and J. P. Eckmann, *Iterated Maps on the Interval as Dynamical Systems* (Birkhäuser, Boston, 1980).
54. R. B. Griffiths, *Phys. Rev. Lett.* **23**:17 (1969).
55. Th. M. Nieuwenhuizen, *Phys. Rev. Lett.* **63**:1760 (1989).