Finite-size scaling of pseudocritical point distributions in the random transverse-field Ising chain

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We study the distribution of finite-size pseudocritical points in a one-dimensional random quantum magnet with a quantum phase transition described by an infinite randomness fixed point. Pseudocritical points are defined in three different ways: the position of the maximum of the average entanglement entropy, the scaling behavior of the surface magnetization, and the energy of a soft mode. All three lead to a log-normal distribution of the pseudocritical transverse fields, where the width scales as $L^{-1/\nu}$ with $\nu=2$ and the shift of the average value scales as $L^{-1/\nu_{typ}}$ with $\nu_{typ}=1$, which we related to the scaling of average and typical quantities in the critical region.

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I. FINITE-SIZE SCALING IN DISORDERED SYSTEMS

Quenched disorder has a profound effect on the physical characteristics of phase transitions in classical and quantum mechanical systems. A theoretically and experimentally important issue is the measurement of physical observables in disordered systems at or near critical points. These measurements are always performed on finite samples and on one particular realization of disorder. Finite-size scaling[1] (FSS) is the systematic way to extract information on the thermodynamic limit by studying finite systems, and the objects to be analyzed by FSS of disordered systems are the distributions of physical properties in the ensemble of the disorder realizations. This also sheds light on the question of whether a single experimental measurement on a rather large system is representative of the whole ensemble of random systems to which it belongs. This is very much connected to the important issue of self-averaging[2,3] of thermodynamic quantities such as the expectation values for order parameter, specific heat, or susceptibilities.

In an infinite system, these observables display a characteristic singularity at a critical point, where, for instance, the susceptibility diverges. This divergence is suppressed in a finite system and replaced by a finite maximum, the location of which is called pseudocritical point and is slightly shifted against the infinite system's critical point. In pure systems, this shift depends on the lateral system's size L, usually proportional to L^{-1/ν_P}, where ν_P is the correlation length exponent of the pure system. In finite disordered systems, the susceptibility usually has several maxima in the critical region and each one is slightly shifted against the critical point of an infinite system. One identifies the location of the largest maximum with the pseudocritical point of the corresponding sample, and an intriguing question, therefore, concerns the distributions of these pseudocritical points.

If the disorder is irrelevant according to the Harris criterion $\nu_P > 2/d$,[4] d being the dimension of the variation of the disorder (usually identical with the system's spatial dimension), the width of the distribution scales as $L^{-d/2}$. In this case, the shift of the average finite-size transition point is proportional to L^{-1/ν_P}. Consequently, the sample to sample fluctuations are asymptotically negligible compared with the shift of the average value, which is referred to as self-averaging. For relevant disorder $\nu_P < 2/d$, there is a new random (R) fixed point at which the exponent, $\nu_R \neq \nu_P$, satisfies the relation[5] $\nu_R \geqslant 2/d$. In many random systems (diluted magnets, random field problems, spin glasses, etc.), the random fixed point is of conventional form, which means that thermal and disorder fluctuations remain of the same order at large scales, i.e., during renormalization. According to the FSS theory of conventional random critical points,[3] both the shift and the width of the distribution of pseudocritical points are characterized by the same random exponent and there is a lack of self-averaging.[2] These predictions, which have been debated for some time,[6] were checked later for various models.[2,3,7–9]

Recently, a new type of random fixed point, the so-called infinite randomness fixed point, has been observed in various systems (e.g., disordered quantum magnets at $T=0$, random stochastic models, etc.), in which the disorder plays a dominant role over quantum, thermal, or stochastic fluctuations[10] and the strength of disorder grows without limits during renormalization.[11] A paradigmatic model for a random magnet with an infinite randomness fixed point is the random transverse-field Ising spin chain[12] (RTFIC), for which many asymptotically exact results have been obtained, partially by the use of a strong disorder renormalization group (SDRG) method.[10] In this paper, we intend to examine the distribution of pseudocritical points and its FSS for the infinite randomness fixed point of the RTFIC.

In the following section, the model and its basic properties are introduced. The pseudocritical points of the model are determined by three different methods in Sec. III and their distribution is analyzed in Sec. IV. The paper is closed by a discussion.

II. MODEL

The random transverse-field Ising spin chain is defined by the Hamiltonian

$$H = -\sum_l J_l \sigma_l^x \sigma_{l+1}^x - \sum_l h_l \sigma_l^z \tag{1}$$

in terms of the $\sigma_l^{x,z}$ Pauli matrices at site l. Here, the J_l exchange couplings and the h_l transverse fields are independent random variables. We are interested in the properties of the system in its ground state. In the thermodynamic limit, the control parameter is given by[13]

$$\delta = [\ln h]_{\rm av} - [\ln J]_{\rm av}, \tag{2}$$

where $[\cdots]_{\rm av}$ denotes averaging over quenched disorder, so that $\delta=0$ at the critical point.[13] In the following, we consider the case of random couplings J_l and homogeneous transverse fields $h_l=h$,[14] so that h is the analog of the temperature in thermal transitions. Its critical value in the thermodynamic limit is given by $\ln h_c(\infty)=[\ln J]_{\rm av}$. In the vicinity of the critical point, the average correlation length involves the exponent $\nu=2$, whereas the typical correlation length diverges with a different exponent $\nu_{typ}=1$.[11] The characteristic time scale τ, which is related to the smallest gap as $\tau \sim \epsilon^{-1}$, scales logarithmically at the critical point, $\ln \tau \sim \sqrt{L}$. It remains divergent in an extended region of the off-critical phase, in the so-called Griffiths phase, where $\tau \sim L^z$ with a dynamical exponent $z=z(\delta)$.

FSS of the RTFIC has been studied in Refs. 15–17. The distribution of the surface magnetization could be computed analytically.[16,17] The distribution of the gap,[17,18] the end-to-end spin-correlation function,[17,18] and the end-to-end energy-correlation function[19] has been calculated by the SDRG method, both in the usual "canonical" ensemble, where the disorder variables are independent, and in the so-called microcanonical ensemble, where there exists a global constraint on the disorder variables. The distributions of observables turned out to be different in the two ensembles, in particular, in the tails that govern averaged values.

III. CALCULATION OF PSEUDOCRITICAL POINTS

In this section, we define sample dependent critical parameters $h_c(\alpha,L)$ (where α indicates a particular disorder realization) and study their distribution. The standard approach, defining $h_c(\alpha,L)$ through the rounding off of the singularity of the susceptibility, is not feasible for the RTFIC since the susceptibility is divergent also in the Griffiths phase. A similar problem arises for the rounding off of the specific heat due to its weak essential singularity.

A. Pseudocritical points through the maximum of the average entropy

Here, we suggest that for random quantum systems, the pseudocritical transition points can be conveniently defined

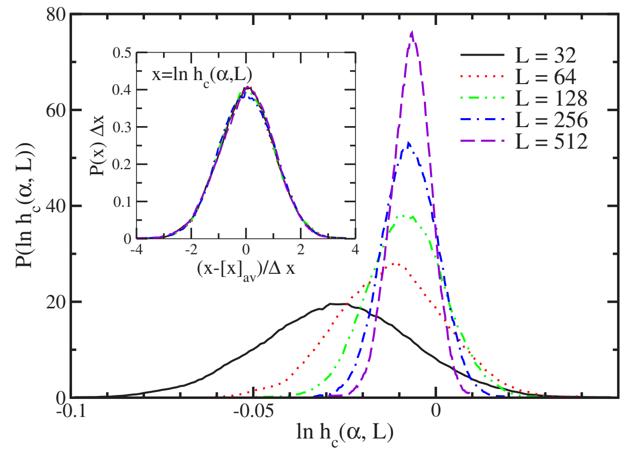

FIG. 1. (Color online) Distribution of $\ln h_c(\alpha,L)$ for a disorder with $\Delta J=0.4$, for different sizes. In the inset, the distributions of scaled variables is well described by a Gaussian.

through the rounding off of the average entanglement entropy. For the RTFIC, we consider a periodic sample (α) of length L and calculate the entanglement entropy between the two halves of the chain, which is then averaged over all possible starting points of the block. In the limit $L \to \infty$, the average entropy is divergent at the critical point,[20] whereas in a finite sample, we use the position of its maximum to define $h_c(\alpha,L)$.

In the numerical calculations, we have used efficient free-fermion techniques[21,22] by which we could calculate the entanglement entropy up to sizes $L=512$. The couplings in Eq. (1) are taken from a uniform boxlike distribution, which is centered at $J=1$ and has a width ΔJ. For different strengths of disorder ($\Delta J=0.2$, 0.4, 0.6, and 1.0) and for each system size L, 10 000 disorder realizations were generated. Additionally, the entropy of each sample is averaged over $L/2$ starting position of the block. As an illustration, we show in Fig. 1 the probability distributions of $\ln h_c(\alpha,L)$ at a disorder $\Delta J=0.4$ for different sizes. The distribution functions for different L are symmetric, and in terms of rescaled variables $(\ln h_c(\alpha,L)-[\ln h_c(\alpha,L)]_{\rm av})/\Delta \ln h_c(\alpha,L)$, the transformed distributions are well fitted by the same Gaussian form, as shown in the inset of Fig. 1. For different strengths of disorder, we have analyzed the shift of the average value, $[\ln h_c(\alpha,L)]_{\rm av}$, as well as that of the standard deviation, $\Delta \ln h_c(\alpha,L)$, which are shown in Fig. 2. Interestingly, the average transition point for a given L is practically independent of the strength of disorder and corresponds to the value in the pure system.

Our numerical data are compatible with a FSS form for the shift that is given by $\ln h_c(\infty)-\ln h_c(L) \sim L^{-a}$, with an effective exponent a which is close to 2 but has a variation with L. Analyzing the data for the pure system, we observed a logarithmic correction: $\ln h_c(\infty)-\ln h_c(L) \sim L^{-2} \ln L$. This unusual combination probably represents the correction to scaling behavior when the prefactor of the expected leading $1/L$ term is vanishing. The scaling of the width of the distributions is found to follow $\Delta \ln h_c(L) \sim L^{-1/\nu}$, where the exponent is given by $1/\nu=0.50(1)$ independent of the strength of disorder (Fig. 2). Thus, our numerical estimate for ν

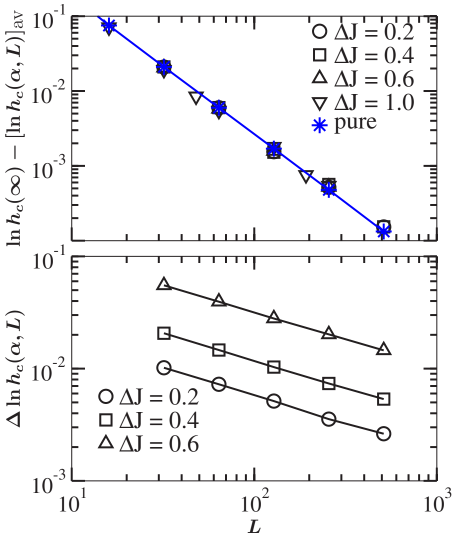

FIG. 2. (Color online) Upper panel: Shift of the average of $\ln h_c(\alpha,L)$ as a function of L in a log-log scale. The data points have practically no disorder dependence. The straight line has a slope of 1.8, which represents an effective exponent close to 2. Lower panel: Scaling of the width of the distribution of $\ln h_c(\alpha,L)$ as a function of L in a log-log scale. The slope of the straight lines is practically disorder independent: $1/\nu=0.50(1)$.

agrees well with the exponent of the average correlation length of the RTFIC.

In the following, we use two other definitions of the sample dependent pseudocritical points, both of which can be worked out analytically. In Sec. III B, we consider the surface magnetization, and in Sec. III C, the energy of a soft mode.

B. Pseudocritical points through the surface magnetization

The surface magnetization is perhaps the simplest physical quantity of the RTFIC. Fixing the spin at one end of the chain, say, at $l=L+1$, which amounts to having $h_{L+1}=0$, the magnetization at the other end of the chain at $l=1$ is given by the exact formula[23]

$$m_s = \left[1 + \sum_{l=1}^{L} \prod_{j=1}^{l} \left(\frac{h_j}{J_j} \right)^2 \right]^{-1/2}. \tag{3}$$

In the following, we use a doubling procedure:[9] For a given random sample (α) of length L, we construct a replicated sample (2α) of length $2L$ by gluing two copies of (α) together, and study the ratio of the surface magnetizations: $r(\alpha,L)=m_s(2\alpha,2L)/m_s(\alpha,L)$. We rewrite the exact expression in Eq. (3) as

$$m_s(\alpha,L) = [Z_1(L)+1]^{-1/2}, \quad Z_1(L) = \sum_{l=1}^{L} e^{-U(l)} \tag{4}$$

in terms of a random walk variable: $U(i)=2\sum_{j=1}^{i} \ln \frac{J_j}{h_j}$. Similarly, we obtain for the replicated sample

$$m_s(2\alpha,2L) = [Z_2(L)+1]^{-1/2}, \quad Z_2(L) = \sum_{l=1}^{2L} e^{-U_2(l)}, \tag{5}$$

where $U_2(i)=U(i)$ for $1 \leqslant i \leqslant L$ and it is $U_2(i)=U(L)+U(i-L)$ for $L+1 \leqslant i \leqslant 2L$. The expression in Eq. (5) simplifies into $Z_2(L)=(1+e^{-U(L)})Z_1(L)$. Since in the critical region $\ln Z_1(L) \sim L^{1/2}$ for large L, the ratio of the two surface magnetizations is given by

$$r(\alpha,L) \simeq (1+e^{-U(L)})^{-1/2}. \tag{6}$$

For the pure chain in the ordered phase with $\delta_P=h-h_c(\infty)=h-1<0$, we have $U(L)\to\infty$, whereas in the disordered phase it is $U(L)\to-\infty$. Then at the critical point, $U(L)=0$ and the ratio has a nontrivial value, $r(L)=1/\sqrt{2}$. For the random chain, we have the same type of trivial fixed points and it is natural to use the condition $U(L)=0$ to define finite-size critical transverse fields. This leads to the microcanonical condition:

$$\frac{1}{L}\sum_{l=1}^{L} \ln J_l = \frac{1}{L}\sum_{l=1}^{L} \ln h_l = \ln h_c(\alpha,L). \tag{7}$$

Using this definition, we obtain for the finite-size behavior in the disordered phase for a given sample $\ln m_s(\alpha,L) \sim -[\ln h_c(\alpha,L)-\ln h]L$, and for its average, $[\ln m_s(\alpha,L)]_{\rm av} \sim -[\ln h_c(\infty)-\ln h]L \sim -|\delta|L$, which involves the typical exponent, $\nu_{typ}=1$.

C. Pseudocritical points through a soft mode

Criticality of the RTFIC in the free-fermion representation is related to the vanishing of the excitation energy of a special fermionic mode. We recall that for closed chains, i.e., with $J_L \neq 0$, the even and odd numbers of excitations are taken from two different sectors: the ground state is the vacuum of the even sector, whereas the first excited state is in the odd sector and contains one fermion with energy Λ_1. For the pure system, its energy is given by $\Lambda_1^P=h-J=\delta_P$; thus, it changes sign at the critical point. Here, we use the same condition, $\Lambda_1=0$, to define criticality in a finite random system, too. This leads to the matrix equation[21] $(\mathbf{A}+\mathbf{B})\mathbf{\Phi}_1=\mathbf{0}$ with

$$(\mathbf{A}+\mathbf{B}) = \begin{pmatrix} h_1 & J_1 & & & & \\ & h_2 & J_2 & & & \\ & & h_3 & J_3 & & \\ & & & \ddots & \ddots & \\ & & & & h_{L-1} & J_{L-1} \\ J_L & & & & & h_L \end{pmatrix}, \tag{8}$$

the solution of which is just the microcanonical condition in Eq. (7).

In the following, we study the scaling behavior of the smallest gap $\epsilon(\alpha,L)$ in the ordered phase. For this it is more convenient to use open chains with L bonds where we have the asymptotic expression[15]

$$\epsilon(\alpha,L) \sim m_s(\alpha,L)\overline{m_s}(\alpha,L)\prod_{i=1}^{L}\frac{h_i}{J_i}h_1, \qquad (9)$$

provided the scaled gap, $\epsilon(\alpha,L)L$, goes to zero. Here, we take $h_{L+1}=h_1$. $m_s(\alpha,L)$ and $\overline{m_s}(\alpha,L)$ denote the surface magnetization at the two ends of the chain, which are both $O(\delta^{1/2})$ in the ordered phase,[11,12] since here average and typical values are in the same order. Consequently, for a given sample we have $\ln \epsilon(\alpha,L) \sim -[\ln h - \ln h_c(\alpha,L)]L$, and for its average, $[\ln \epsilon(\alpha,L)]_{av} \sim -[\ln h - \ln h_c(\infty)]L \sim -\delta L$. Thus the finite-size correction involves the typical exponent, $\nu_{typ}=1$.

IV. LOG-NORMAL DISTRIBUTION

We have used three different methods to determine pseudocritical points, all of which give coherent results for the pseudocritical point distributions. We have found that the distribution of $x=\ln h_c(\alpha,L)$ is Gaussian around $\bar{x}=[\ln h_c(\alpha,L)]_{av}$, given by

$$P_L(x=\ln h_c(\alpha,L)) = \sqrt{\frac{L}{2\pi\sigma^2}}e^{-(L/2\sigma^2)(x-\bar{x})^2}. \qquad (10)$$

Thus $\Delta \ln h_c(\alpha,L)=\sigma/\sqrt{L}$, and the fluctuations are governed by the exponent $\nu=2$. The shift of the average, $\ln h_c(\infty)-\bar{x}$, is of $O(L^{-2}\ln L)$ from the average entropy and zero by the other two methods. The average of the critical transverse fields is given by $[h_c(\alpha,L)]_{av}=e^{\bar{x}}e^{\sigma^2/2L}=h_c(\infty)(1+2\sigma^2/L+\cdots)$, leading to $[h_c(\alpha,L)]_{av}-h_c(\infty)\sim 1/L$, which is consistent with $\nu_{typ}=1$. We can, thus, conclude that

$$\frac{\Delta h_c(L)}{[h_c(\alpha,L)]_{av}-h_c(\infty)} \sim \sqrt{L}, \qquad (11)$$

which tends to infinity as $L\to\infty$. This property can be taken as a definition of an infinite randomness fixed point.

We now use these results to explain the role of the averaged correlation length δ^{-2}. In the disordered phase $[h>h_c(\infty)]$, the average surface magnetization $[m_s(h,L)]_{av}$ is dominated by the rare ordered samples having $m_s(\alpha,L)=O(1)$, for which $h_c(\alpha,L)>h>h_c(\infty)$. From their probability, we obtain

$$[m_s(h,L)]_{av} \sim \text{Prob}(\ln h_c(\alpha,L) > \ln h) \sim e^{-(L/2\sigma^2)\delta^2}. \qquad (12)$$

Its exponential decay, thus, involves the critical exponent $\nu=2$. In the ordered phase $[h<h_c(\infty)]$, we consider the average gap, $[\epsilon(h,L)]_{av}$, which is dominated by those rare realizations, for which $h_c(\alpha,L)<h<h_c(\infty)$ and $\epsilon(\alpha,L)=O(1)$. From their probability, we obtain

$$[\epsilon(h,L)]_{av} \sim \text{Prob}(\ln h_c(\alpha,L) < \ln h) \sim e^{-(L/2\sigma^2)\delta^2}, \qquad (13)$$

which also involves the critical exponent $\nu=2$. We note that previously we have shown that the typical quantities, both the surface magnetization and the gap, have an exponential decay: $e^{-L|\delta|}$, involving the typical exponent, $\nu_{typ}=1$.

V. DISCUSSION

In this paper, we have studied the distribution of the pseudocritical points of the RTFIC and obtained exact results. While the shift of the average transition points scales with the exponent of the typical correlation length, the scaling of the width of the distribution involves the average correlation length exponent. This latter quantity plays a dominant role, as shown in Eq. (11). The investigations presented in this paper can be extended for another random system displaying an infinite randomness fixed point. For random quantum spin chains, e.g., for the random antiferromagnetic Heisenberg and *XX* chains in the presence of dimerization, one can use the positions of the maximum entropy, as presented in Sec. III A, to define the pseudocritical points. In higher dimensional realizations of infinite randomness fixed points, like the two-dimensional random transverse-field Ising model,[24,25] one can calculate the entropy numerically by the SDRG method[26] and then use the maximum entropy to locate the pseudocritical points. Various stochastic models with quenched disorder also display an infinite randomness fixed point, examples include the Sinai walk and the partially asymmetric exclusion process.[10] In these models, the pseudocritical point of the sample is identified with the vanishing of the average velocity or the current. In each case, we expect that for the distribution of the pseudocritical points, the same scenario as discussed in this paper holds: in the scaling, two correlation length exponents are involved and the width of the distribution is dominant over the shift of the average value.

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