

Finite-temperature and dynamical properties of the random transverse-field Ising spin chain

A. P. Young

Department of Physics, University of California, Santa Cruz, California 95064

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We study numerically the paramagnetic phase of the spin-1/2 random transverse-field Ising chain, using a mapping to noninteracting fermions. We extend our earlier work, Phys. Rev. B **53**, 8486 (1996), to finite temperatures and to dynamical properties. Our results are consistent with the idea that there are Griffiths-McCoy singularities in the paramagnetic phase described by a continuously varying exponent $z(\delta)$, where δ measures the deviation from criticality. There are some discrepancies between the values of $z(\delta)$ obtained from different quantities, but this may be due to corrections to scaling. The *average* on-site time dependent correlation function decays with a power law in the paramagnetic phase, namely, $\tau^{-1/z(\delta)}$, where τ is imaginary time. However, the *typical* value decays with a stretched exponential behavior, $\exp(-c\tau^{1/\mu})$, where μ may be related to $z(\delta)$. We also obtain results for the full probability distribution of time dependent correlation functions at different points in the paramagnetic phase. [S0163-1829(97)07641-8]

I. INTRODUCTION

Most critical points occur at a finite temperature and one tunes through the transition by varying the temperature itself. There are however, many critical points which occur at zero temperature and are traversed by varying some other parameter. These quantum critical points have recently been of great interest, particularly for systems with disorder. One reason for this interest is that even the paramagnetic phase can have quite dramatic singularities. For example, in systems with a discrete symmetry, such as the Ising model discussed in this paper, there is a line in the phase diagram, on either side of the critical point, where correlations in time (but not in space) decay with a power law.¹⁻³ Power law behavior is characteristic of a critical point, but here this critical-like behavior occurs only in the time direction. We could say that there is a line of "semicritical" points. Furthermore, the exponent characterizing the power law decay is expected to vary continuously along the line.¹⁻⁴ As a result static response functions may actually *diverge* in a finite region away from the critical point.²⁻⁵

These singularities arise from regions of the sample which have stronger interactions than average and were first discussed, many years ago, by Griffiths,⁶ in the context of *classical* models, where, however, they are rather weak.⁷ At about the same time, McCoy⁵ determined exactly some properties of a two-dimensional classical model (equivalent to the disordered one-dimensional quantum magnet that we study here), finding that the susceptibility diverges before the critical point is reached. It is now understood that this behavior is due the rare regions, more strongly coupled than average, discussed by Griffiths, but which give a larger effect in the quantum regime than near a classical transition. Hence we shall refer to Griffiths singularities in the quantum regime as Griffiths-McCoy singularities.

We shall study here the disordered spin-1/2 Ising chain in one dimension, for which many properties can be worked out in detail. The ground state of this model is closely related to the finite-temperature behavior of a two-dimensional classical Ising model with disorder perfectly correlated along one

direction, which was first studied by McCoy⁵ and by McCoy and Wu.⁸ Subsequently, the quantum model was studied by Shankar and Murthy⁹ and, in great detail, by Fisher.⁴ From a real space renormalization group analysis, which becomes exact on large scales, Fisher obtained many results and considerable physical insight. One of the key conclusions is that many quantities have very broad distributions, with average and typical values being quite different. Consequently, a lot of information is lost by averaging. Confirmation of Fisher's surprising predictions for the $T=0$, equal time behavior of the quantum problem, as well as some results for distributions of various quantities, were obtained in an earlier work¹⁰ (henceforth denoted by YR), which used a mapping of the spin problem to noninteracting fermions¹¹⁻¹³ to obtain accurate numerical results for quite large systems.

In this paper we extend these techniques to finite temperatures and finite times. Our data suggest that the singularities are governed by a continuously varying exponent, though there are some discrepancies which we discuss. We also obtain results for the *distribution* of time dependent correlation functions, showing, for example, that a *typical* correlation function decays with a stretched exponential dependence on time, as opposed to the average which decays with a power, as noted above. Recently, results for dynamical correlations at the critical point have been obtained by Rieger and Igloi¹⁴ using similar techniques to ours. Hence our results will be restricted to the paramagnetic phase.

II. THE MODEL

The model that we study is one-dimensional random transverse-field Ising chain with Hamiltonian

$$\mathcal{H} = - \sum_{i=1}^{L-1} J_i \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^L h_i \sigma_i^x. \quad (1)$$

Here the $\{\sigma_i^\alpha\}$ are Pauli spin matrices, and the interactions J_i and transverse fields h_i are both independent random variables, with distributions $\pi(J)$ and $\rho(h)$, respectively. The lattice size is L , and, in this paper, we will take *free*, rather

than the more usual periodic, boundary conditions. We will see later why this is necessary.

Since the model is in one dimension, we can perform a gauge transformation to make all the J_i and h_i positive. Unless otherwise stated, the numerical work used the following rectangular distribution:

$$\pi(J) = \begin{cases} 1 & \text{for } 0 < J < 1, \\ 0 & \text{otherwise,} \end{cases}$$

$$\rho(h) = \begin{cases} h_0^{-1} & \text{for } 0 < h < h_0, \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

The model is therefore characterized by a single control parameter, h_0 . Defining

$$\Delta_h = [\ln h]_{\text{av}},$$

$$\Delta_J = [\ln J]_{\text{av}}, \quad (3)$$

where $[\dots]_{\text{av}}$ denote an average over disorder, the critical point occurs when^{9,4}

$$\Delta_h = \Delta_J. \quad (4)$$

Clearly this is satisfied if the distributions of bonds and fields are equal, and the criticality of the model then follows from duality.⁴ A convenient measure of the deviation from criticality is given by⁴

$$\delta = \frac{\Delta_h - \Delta_J}{\text{var}(\ln h) + \text{var}(\ln J)}, \quad (5)$$

where $\text{var}(\dots)$ denotes the variance. For the distribution in Eq. (2), we have

$$\delta = \frac{1}{2} \ln h_0. \quad (6)$$

III. THE METHOD

The numerical technique for static quantities, has been discussed in detail for periodic boundary conditions by YR. Here we consider free boundary conditions, which is simpler, so we will only summarize the main results. Following Lieb, Schultz, and Mattis¹¹ we start by using the the Jordan-Wigner transformation, which relates the spin operators to fermion creation and annihilation operators, c_i^\dagger and c_i :

$$\sigma_i^z = a_i^\dagger + a_i,$$

$$\sigma_i^y = i(a_i^\dagger - a_i),$$

$$\sigma_i^x = 1 - 2a_i^\dagger a_i = 1 - 2c_i^\dagger c_i, \quad (7)$$

where

$$a_i^\dagger = c_i^\dagger \exp\left[-i\pi \sum_{j=1}^{i-1} c_j^\dagger c_j\right],$$

$$a_i = \exp\left[-i\pi \sum_{j=1}^{i-1} c_j^\dagger c_j\right] c_i. \quad (8)$$

The Hamiltonian, Eq. (1), can then be written¹⁵

$$\mathcal{H} = \sum_{i=1}^L h_i (c_i^\dagger c_i - c_i c_i^\dagger) - \sum_{i=1}^{L-1} J_i (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}). \quad (9)$$

Note that the fermion Hamiltonian, Eq (9), is bilinear and so describes *free* fermions.

We define operators Ψ_j^\dagger for $1 \leq j \leq 2L$ by $\Psi_i^\dagger = c_i^\dagger$ and $\Psi_{i+L}^\dagger = c_i$, where $1 \leq i \leq L$. Similarly Ψ_i is the Hermitian conjugate of Ψ_i^\dagger . Note that the Ψ_i and Ψ_j^\dagger satisfy the usual fermion commutation relations for *all* i and j .

The Hamiltonian, Eq (9), can then be written in terms of a real-symmetric $2L \times 2L$ matrix, \tilde{H} , as

$$\mathcal{H} = \Psi^\dagger \tilde{H} \Psi, \quad (10)$$

where \tilde{H} has the form

$$\tilde{H} = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}, \quad (11)$$

where A and B are $L \times L$ matrices with elements

$$A_{i,i} = h_i,$$

$$A_{i,i+1} = -J_i/2,$$

$$A_{i+1,i} = -J_i/2,$$

$$B_{i,i+1} = J_i/2,$$

$$B_{i+1,i} = -J_i/2, \quad (12)$$

where, since we have free boundary conditions, elements with an index $L+1$ are zero. Note that \tilde{H} is real symmetric.

Next we diagonalize \tilde{H} numerically, to find the single-particle eigenstates with eigenvalues $\epsilon_\mu/2$, $\mu = 1, 2, \dots, 2L$ and eigenvectors Φ_μ^\dagger which are linear combinations of the Ψ_i^\dagger with real coefficients.¹⁶ It is easy to see that the eigenstates come in pairs, with eigenvectors that are Hermitian conjugates of each other and eigenvalues which are equal in magnitude and opposite in sign. We can therefore define $\Phi_\mu^\dagger = \gamma_\mu^\dagger$ if $\epsilon_\mu > 0$ and $\Phi_{\mu'}^\dagger = \gamma_{\mu'}$ if μ' is the state with energy $-\epsilon_\mu$.

The Hamiltonian can then be written just in terms of L (rather than $2L$) modes as

$$\mathcal{H} = \frac{1}{2} \sum_{\mu=1}^L \epsilon_\mu (\gamma_\mu^\dagger \gamma_\mu - \gamma_\mu \gamma_\mu^\dagger)$$

$$= \sum_{\mu=1}^L \epsilon_\mu \left(\gamma_\mu^\dagger \gamma_\mu - \frac{1}{2} \right), \quad (13)$$

where all the ϵ_μ are now taken to be positive. The average energy per site is therefore given by

$$E_{\text{av}} = \frac{1}{L} \sum_{\mu=1}^L \left[\epsilon_\mu \left(n_\mu - \frac{1}{2} \right) \right]_{\text{av}}, \quad (14)$$

where n_μ is the Fermi function,

$$n_\mu = \frac{1}{\exp(\beta \epsilon_\mu) + 1}, \quad (15)$$

and the specific heat is consequently given by

$$C_{\text{av}} = \frac{1}{LT^2} \sum_{\mu=1}^L [\epsilon_{\mu}^2 n_{\mu} (1 - n_{\mu})]_{\text{av}}, \quad (16)$$

in units where $k_B = 1$, which we take from now on.

We next consider equal time correlation functions, defined by

$$S_{ij} = \langle \sigma_i^z \sigma_j^z \rangle. \quad (17)$$

Since $S_{ji} = S_{ij}$, we can take $j > i$, without loss of generality. S_{ij} is given in terms of a determinant of size $j - i$ by¹¹

$$S_{ij} = \begin{vmatrix} G_{i,i+1} & G_{i,i+2} & \cdots & G_{ij} \\ G_{i+1,i+1} & G_{i+1,i+2} & \cdots & G_{i+1,j} \\ \vdots & \vdots & \ddots & \vdots \\ G_{j-1,i+1} & G_{j-1,i+2} & \cdots & G_{j-1,j} \end{vmatrix}, \quad (18)$$

where

$$G_{ij} = \langle (c_i^{\dagger} - c_i)(c_j^{\dagger} + c_j) \rangle. \quad (19)$$

G_{ij} can be expressed in terms of the eigenvectors of the matrix \tilde{H} in Eq. (11). Let us write

$$\begin{aligned} c_i^{\dagger} + c_i &= \sum_{\mu=1}^L \phi_{\mu i} (\gamma_{\mu}^{\dagger} + \gamma_{\mu}), \\ c_i^{\dagger} - c_i &= \sum_{\mu=1}^L \psi_{\mu i} (\gamma_{\mu}^{\dagger} - \gamma_{\mu}), \end{aligned} \quad (20)$$

where ψ and ϕ can be shown to be orthogonal matrices. Then

$$\begin{aligned} G_{ij} &= \langle (c_i^{\dagger} - c_i)(c_j^{\dagger} + c_j) \rangle \\ &= \sum_{\mu=1}^L \psi_{\mu i} \phi_{\mu j} \langle (\gamma_{\mu}^{\dagger} - \gamma_{\mu})(\gamma_{\mu}^{\dagger} + \gamma_{\mu}) \rangle \\ &= - \sum_{\mu=1}^L (\psi^T)_{i\mu} (1 - 2n_{\mu}) \phi_{\mu j}, \end{aligned} \quad (21)$$

since

$$\langle \gamma_{\mu}^{\dagger} \gamma_{\mu}^{\dagger} \rangle = \langle \gamma_{\mu} \gamma_{\mu} \rangle = 0, \quad (22)$$

$$\langle \gamma_{\mu}^{\dagger} \gamma_{\mu} \rangle = 1 - \langle \gamma_{\mu} \gamma_{\mu}^{\dagger} \rangle = n_{\mu}. \quad (23)$$

At zero temperature, Eq. (21) goes over to Eq. (54) of YR.

We now discuss how these results are generalized to time dependent correlation functions.^{17,18} We are interested in the σ^x - σ^z imaginary time¹⁹ correlation function, $S_{ij}(\tau)$ for $0 \leq \tau \leq \beta$, where

$$S_{ij}(\tau_1 - \tau_2) = \langle \sigma_i^z(\tau_1) \sigma_j^z(\tau_2) \rangle, \quad (24)$$

with

$$\sigma_i^z(\tau_1) = e^{\tau_1 \mathcal{H}} \sigma_i^z e^{-\tau_1 \mathcal{H}}. \quad (25)$$

Note that

$$S_{ij}(\tau) = S_{ji}(\beta - \tau), \quad (26)$$

which follows by cyclically permuting the trace, and so, without loss of generality, we just consider $j \geq i$.

Substituting the transformation in Eq. (8) one has

$$\begin{aligned} S_{ij}(\tau) &= \left\langle \exp \left[-i\pi \sum_{m=1}^{i-1} c_m^{\dagger}(\tau) c_m(\tau) \right] [c_i^{\dagger}(\tau) + c_i(\tau)] \right. \\ &\quad \left. \times \exp \left[-i\pi \sum_{l=1}^{j-1} c_l^{\dagger} c_l \right] (c_j^{\dagger} + c_j) \right\rangle. \end{aligned} \quad (27)$$

This can be simplified since

$$\exp[-i\pi c_m^{\dagger} c_m] = A_m B_m, \quad (28)$$

where

$$\begin{aligned} A_m &= c_m^{\dagger} + c_m, \\ B_m &= c_m^{\dagger} - c_m, \end{aligned} \quad (29)$$

and so

$$S_{ij}(\tau) = \left\langle \left(\prod_{m=1}^{i-1} A_m(\tau) B_m(\tau) \right) A_i(\tau) \left(\prod_{l=1}^{j-1} A_l B_l \right) A_j \right\rangle. \quad (30)$$

Hence $S_{ij}(\tau)$ involves the product of $2(i+j-1)$ Fermi operators. This number is very large if one is interested in two sites near the center of a large lattice, even if those sites are close together.

The situation is much simpler for $t=0$ because then the product of all the operators to the left of site i is unity,²⁰ and so

$$S_{ij}(0) = \left\langle A_i \left[\prod_{l=i}^{j-1} A_l B_l \right] A_j \right\rangle = \left\langle B_i \left[\prod_{l=i+1}^{j-1} A_l B_l \right] A_j \right\rangle, \quad (31)$$

where the last line follows because $A_i^2 = 1$. As shown by Lieb *et al.*,¹¹ Wick's theorem, together with the observation that

$$\langle A_i A_j \rangle = -\langle B_i B_j \rangle = \delta_{ij}, \quad (32)$$

enables one to write $S_{ij}(t=0)$ as the Toeplitz determinant of order $j-i$ in Eq. (18). This is convenient because the determinant is small if i and j are close together, even for sites far from the boundary of a large system.

For $\tau \neq 0$ in Eq. (30) one can still use Wick's theorem but now there are many more pairs of operators to be included in the contractions. Wick's theorem for fermions requires the sum over all possible products of pair averages, with a sign which is 1 or -1 depending on whether an even or odd permutation of the operators is necessary to get the operators in the product back to the original order. This is called a Pfaffian; see, e.g., the book by McCoy and Wu.²¹ If the number of operators $2n$ is large (here $n = i + j - 1$), evaluation of the Pfaffian is intractable because the number of terms $(2n-1)!!$ is too large even for fast computers. However, the Pfaffian is also the square root of an antisymmetric matrix (of order $2n$) formed from the pair averages. To be precise, if A, B, \dots, Z are Fermi operators, and the average is over a free Fermi Hamiltonian (in the grand canonical ensemble), one has²¹

$$\langle ABC \cdots Z \rangle = \begin{vmatrix} 0 & \langle AB \rangle & \langle AC \rangle & \cdots & \langle AZ \rangle \\ -\langle AB \rangle & 0 & \langle BC \rangle & \cdots & \langle BZ \rangle \\ -\langle AC \rangle & -\langle BC \rangle & 0 & \cdots & \langle CZ \rangle \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\langle AZ \rangle & -\langle BZ \rangle & -\langle CZ \rangle & \cdots & 0 \end{vmatrix}^{1/2} \quad (33)$$

As a simple example, consider $i=1, j=2$ in Eq. (30) for which Wick's theorem gives

$$\begin{aligned} S_{1,2}(\tau) &= \langle A_1(\tau) A_1 B_1 A_2 \rangle \\ &= \langle A_1(\tau) A_1 \rangle \langle B_1 A_2 \rangle - \langle A_1(\tau) B_1 \rangle \langle A_1 A_2 \rangle \\ &\quad + \langle A_1(\tau) A_2 \rangle \langle A_1 B_1 \rangle. \end{aligned} \quad (34)$$

This is easily shown to equal

$$\begin{vmatrix} 0 & \langle A_1(\tau) A_1 \rangle & \langle A_1(\tau) B_1 \rangle & \langle A_1(\tau) A_2 \rangle \\ -\langle A_1(\tau) A_1 \rangle & 0 & \langle A_1 B_1 \rangle & \langle A_1 A_2 \rangle \\ -\langle A_1(\tau) B_1 \rangle & -\langle A_1 B_1 \rangle & 0 & \langle B_1 A_2 \rangle \\ -\langle A_1(\tau) A_2 \rangle & -\langle A_1 A_2 \rangle & -\langle B_1 A_2 \rangle & 0 \end{vmatrix}^{1/2} \quad (35)$$

which is just Eq. (33) for this case. Note that Eq. (32) gives $\langle A_1 A_2 \rangle = 0$ and we also have $A_1^2 = 1$. Hence, for $\tau=0$, we get, from Eq. (34), the simpler result

$$S_{1,2}(0) = \langle B_1 A_2 \rangle, \quad (36)$$

which also follows immediately from Eq. (18).

It is much more convenient to work evaluate the determinant and take the square root than to directly evaluate the Pfaffian. In numerical work, the number of operations required to evaluate the determinant is of order $(2n)^3$, which, for n a few hundred, is feasible, whereas the $(2n-1)!!$ operations to evaluate the Pfaffian is definitely not.

The pair averages needed for Wick's theorem can be evaluated in the same manner used to derive Eq. (21) above for the equal time correlation functions. The result is

$$\begin{aligned} \langle A_i(\tau_1) B_j(\tau_2) \rangle &= \sum_{\mu=1}^L (\phi^T)_{i\mu} [-U_\mu(\tau) + V_\mu(\tau)] \psi_{\mu j}, \\ \langle B_i(\tau_1) A_j(\tau_2) \rangle &= \sum_{\mu=1}^L (\psi^T)_{i\mu} [U_\mu(\tau) - V_\mu(\tau)] \phi_{\mu j}, \\ \langle A_i(\tau_1) A_j(\tau_2) \rangle &= \sum_{\mu=1}^L (\phi^T)_{i\mu} [U_\mu(\tau) + V_\mu(\tau)] \phi_{\mu j}, \\ \langle B_i(\tau_1) B_j(\tau_2) \rangle &= \sum_{\mu=1}^L (\psi^T)_{i\mu} [-U_\mu(\tau) - V_\mu(\tau)] \psi_{\mu j}, \end{aligned} \quad (37)$$

where

$$U_\mu(\tau) = n_\mu e^{\epsilon_\mu \tau},$$

$$V_\mu(\tau) = (1 - n_\mu) e^{-\epsilon_\mu \tau}, \quad (38)$$

and $\tau = \tau_1 - \tau_2$. From these pair averages the determinant in Eq. (33) [with the operators in Eq. (30)] is evaluated numerically, and finally the square root taken. Since the imaginary time correlation function is real and positive, there is no ambiguity about the sign.

We concentrate on the local correlation function, $S_{ii}(\tau)$. This determines the local susceptibility from

$$\chi_{ii} = \int_0^\beta S_{ii}(\tau) d\tau. \quad (39)$$

We determine $S_{ii}(\tau)$ for different values of τ , increasing in a roughly logarithmic manner, and approximate the integral by the trapezium rule. We compute the average local correlation function and average local susceptibility, defined by

$$S_{av}(\tau) = \frac{1}{L} \sum_i [S_{ii}(\tau)]_{av}, \quad \chi_{av}^{loc} = \frac{1}{L} \sum_i [\chi_{ii}]_{av}. \quad (40)$$

From now on, for compactness of notation, we will denote $S_{ii}(\tau)$ by $S(\tau)$. In addition, because there are large fluctuations in the values of $S(\tau)$ from site to site, we also look at the distributions of this quantity for different τ .

IV. PHENOMENOLOGICAL DESCRIPTION

From recent work,^{1-4,10,14} a phenomenological description of the Griffiths-McCoy region of the paramagnetic phase has emerged. Singularities arise from small regions which are "locally in the ferromagnetic phase" and have a very small energy gap. As a result, there are low energy "cluster" excitations, which have a power law distribution of energies, ΔE . The probability of having a low energy excitation is proportional to the size, L , and so we can write the dimensionless probability, $\Delta EP(\Delta E)$, as

$$\Delta EP(\Delta E) \sim L(\Delta E)^{1/z(\delta)}, \quad (41)$$

where we write the power in terms of a dynamical exponent $z(\delta)$, since Eq. (41) corresponds to the standard relation between a length scale (L here) and an energy scale (ΔE here). The exponent is expected to vary continuously in the Griffiths-McCoy phase, and we indicate this by the notation, $z(\delta)$.

For the distribution used here, Eq. (2), in the limit $\delta \rightarrow \infty$ we can neglect the interactions and the excitation energy of a single spin is just $2h_i$. Since the h_i have a uniform distribution for $h \rightarrow 0$, it follows that $z=1$ in this limit, i.e.,

$$\lim_{\delta \rightarrow \infty} z(\delta) = 1. \quad (42)$$

Furthermore, it has been established^{4,9} that $z(\delta) \rightarrow \infty$ at the critical point, i.e.,

$$\lim_{\delta \rightarrow 0} z(\delta) = \infty. \quad (43)$$

The energy per site at low temperature can be estimated from the energy of the excited clusters, i.e.,

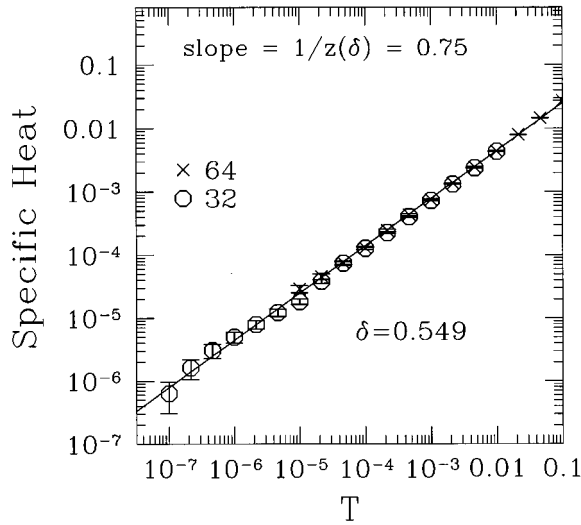


FIG. 1. The specific heat as a function of T for $\delta=0.549$ ($h_0=3$) and sizes $L=64$ and 32 . According to Eq. (45), the slope is $1/z(\delta)$.

$$E_{\text{av}}(T) - E_{\text{av}}(0) \approx \frac{1}{L} \int \Delta E P(\Delta E) \frac{\exp(-\beta \Delta E)}{1 + \exp(-\beta \Delta E)} \sim T^{1+1/z(\delta)}, \quad (44)$$

so the specific heat varies as

$$C_{\text{av}} \sim T^{1/z(\delta)}, \quad (45)$$

for $T \rightarrow 0$.

For a site in a cluster with a low energy excitation ΔE , the long time behavior of $S(\tau)$ is $\exp(-\Delta E \tau)$. Averaging over the distribution gives

$$S_{\text{av}}(\tau) \sim \frac{1}{\tau^{1/z(\delta)}}, \quad (46)$$

and integrating τ up to β gives

$$\chi_{\text{av}}^{\text{loc}} \sim T^{-1+1/z(\delta)}, \quad (47)$$

for $T \rightarrow 0$.

To our knowledge, not much is known about the distribution of $S(\tau)$ and one of the goals of the present work is to deduce its form. Note that because we expect the distribution to be very broad, with average and typical values quite different, we cannot predict its form simply from knowing the average.

V. RESULTS

We start with our results for the specific heat. The data for $h_0=3$ ($\delta=0.549$), shown in Fig. 1, have good straight line behavior for more than five decades; the slope, equal to $1/z(\delta)$, is 0.74.

According to Eq. (42) $z(\delta)$ should tend to unity as $\delta \rightarrow \infty$. This is confirmed by the data for the specific heat for $h=50$ ($\delta=1.956$), shown in Fig. 2, which has a slope of 0.99, very close to the expected value.

The temperature dependence of the susceptibility is shown in Fig. 3 for $h_0=2$ ($\delta=0.346$). Again a power law

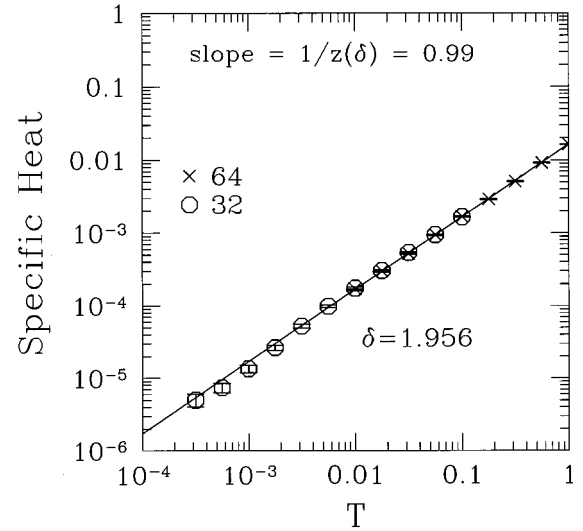


FIG. 2. The specific heat as a function of T for $\delta=1.956$ ($h_0=50$) and sizes $L=64$ and 32 . According to Eqs. (45) and (42), the slope should be close to unity, as indeed it is.

behavior is obtained, as expected from Eq. (47).

We now proceed to our results for the time dependent correlation functions. Data for $S_{\text{av}}(\tau)$ for $h_0=2$ and 6 ($\delta=0.346$ and 0.895) at $T=0$ are shown in Figs. 4 and 5 on a double logarithmic scale. The results clearly indicate a power law behavior, as expected from Eq. (46).

From our results for C_{av} and $S_{\text{av}}(\tau)$, we obtain $z(\delta)$ from Eqs. (45) and (46). We summarize²² these results in Fig. 6. While the trend in the two sets of data is the same, there are some differences, which we do not understand very well. The lattice sizes used are quite large and the data used to generate the estimates for $z(\delta)$ fit a straight line over a fairly large range, especially for the specific heat. This suggests that the estimates for $z(\delta)$ should agree well. However, corrections to scaling may be large because free boundary conditions are used here, as opposed to the more conventional periodic boundary conditions.

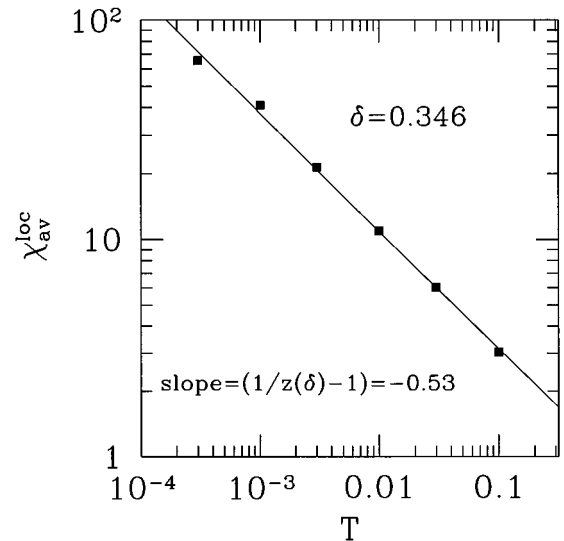


FIG. 3. The susceptibility heat as a function of T for $\delta=0.346$ and size $L=64$.

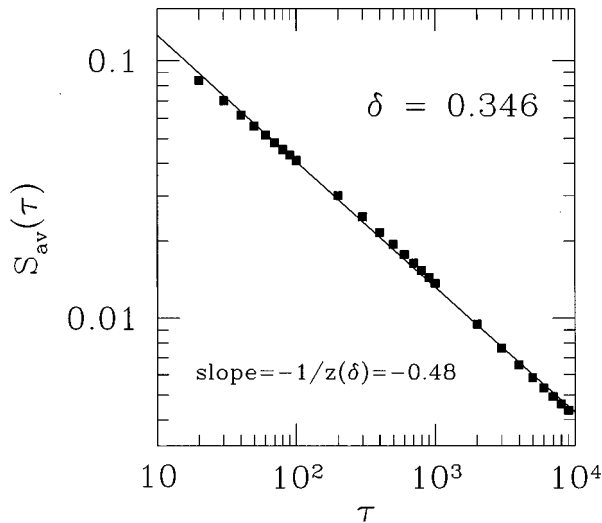


FIG. 4. The average on-site (imaginary) time dependent correlation function at $T=0$ for $\delta=0.346$. The lattice size is $L=64$.

Figure 7 shows the distribution of $\ln S(\tau)$ for $\delta=0.895$. The distribution is broad and becomes broader with increasing τ . We therefore attempt to collapse the data by plotting it versus the scaling variable

$$x = -\frac{\ln S(\tau)}{\tau^{1/\mu}} \quad (48)$$

with an appropriate choice for μ . We shall see that, at a given value of δ , the distributions of $S(\tau)$ for different times are all given by a *single* scaling function $P(x)$.

Figure 8 shows that the data plotted in this way collapses quite well with the choice $\mu=2.2$. For small x the behavior seems to be close to linear, though the data for small times has a finite intercept, which perhaps vanishes for $\tau \rightarrow \infty$. We shall discuss this again later. Scaling plots for $\delta=0.549$ and 0.346 are shown in Figs. 9 and 10. The values of μ used in these fits are 2.2 and 2.5.

From a variable range hopping analysis, Fisher²³ has argued that μ should be related to $z(\delta)$ by

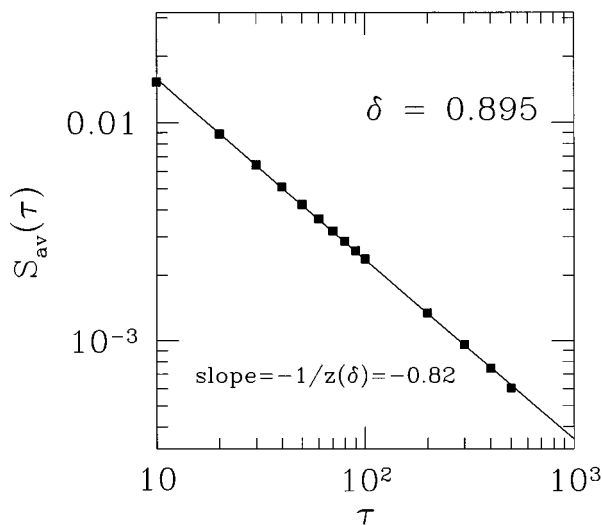


FIG. 5. As for Fig. 4, but with $\delta=0.895$.

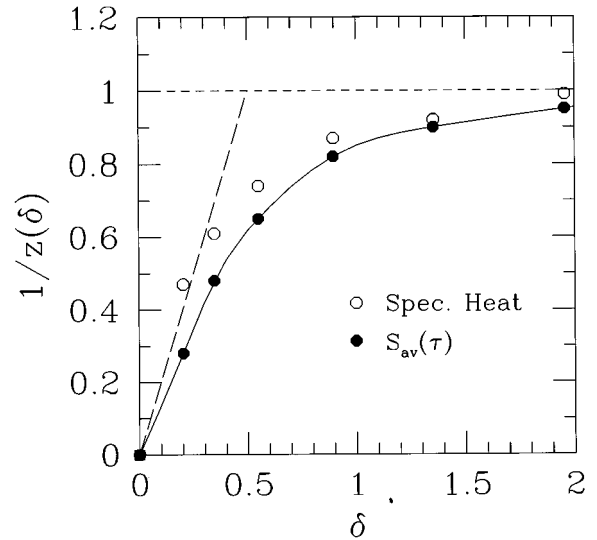


FIG. 6. The dynamic exponent $z(\delta)$ obtained both from the specific heat and the time dependent correlation function. The short-dashed line indicates the asymptotic value $z(\delta \rightarrow \infty)=1$, and the long dashed line is the prediction of Fisher,⁴ $z^{-1}=2\delta$ for $\delta \rightarrow 0$. At the critical point, $\delta=0$, $z(\delta)$ is predicted to be infinite.

$$\mu = 1 + z(\delta). \quad (49)$$

In Appendix A we show that, within the same set of assumptions, the scaling function is given by

$$P(x) = c(cx)^{1/z} \exp\left[-\left(\frac{z}{z+1}\right)(cx)^{(z+1)/z}\right], \quad (50)$$

where

$$x = \frac{-\ln S(\tau)}{\tau^{1/(z+1)}}, \quad (51)$$

as also follows from Eqs. (48) and (49), and c is a scale factor. The data for $\delta=0.895$ fit the scaling function in Eq. (50) quite well, with an appropriate choice of the scale factor

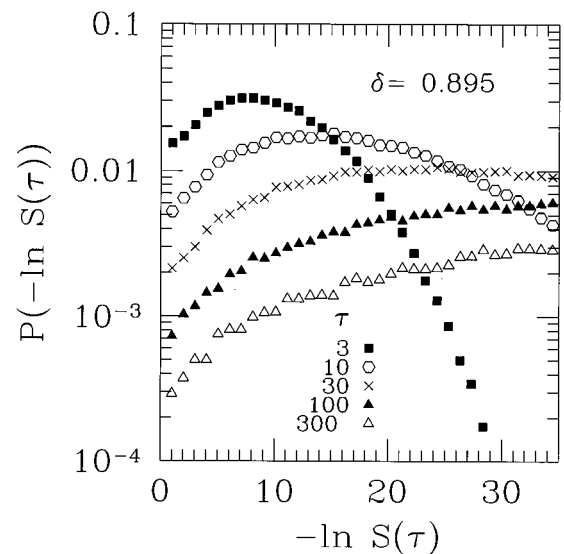


FIG. 7. The distribution of $-\ln S(\tau)$ for $\delta=0.895$. The lattice size is $L=64$ and 50 000 samples were averaged over.

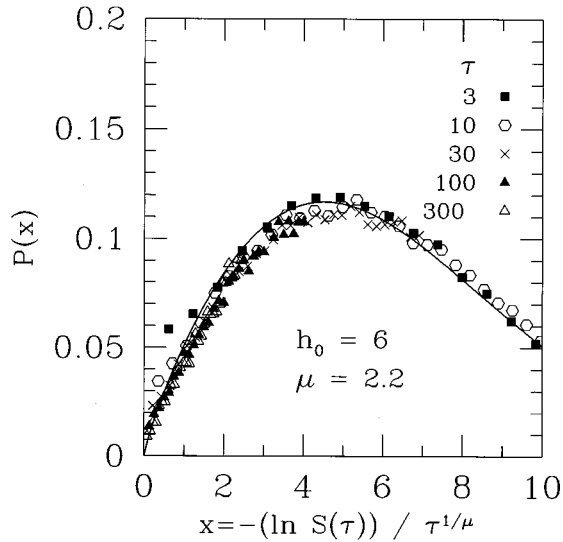


FIG. 8. A scaling plot of the data in Fig. 7. The scaling variable is given in Eq. (48) and we have taken $\mu=2.2$ to get the best fit. The solid line is Eq. (50) with $z=1.2$, consistent with Eq. (49), and $c=0.2$. The fit to the data is good.

c and a value for $z(\delta)$, and hence μ , consistent with that from other data shown in Fig. 6. However, the data closer to the critical point in Figs. 9 and 10 only fit the scaling form if $z(\delta)$ in Eq. (50) and μ in Eq. (48) are adjusted independently. The values for $z(\delta)$ are found to be in reasonable agreement with those in Fig. 6, but the values for μ are then somewhat inconsistent with Eq. (49). Note however, that the stretched exponential is only expected²³ to be valid for times larger than a characteristic time which diverges at the transition. Hence it is possible that our data are not at sufficiently long times for smaller δ to get a good estimate for μ .

The fact that the scaling variable is given by Eq. (48)

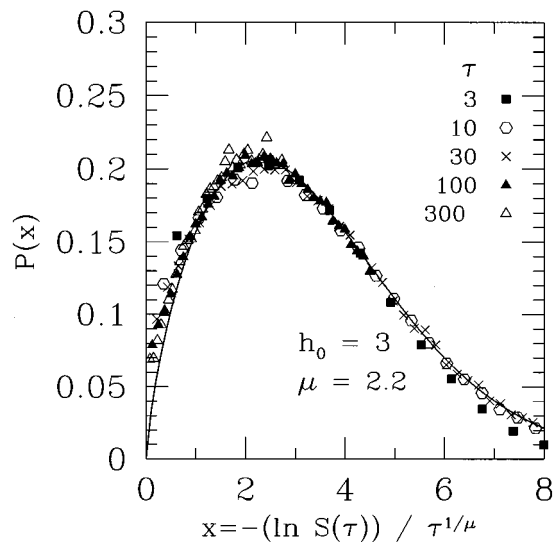


FIG. 9. As for Fig. 8 but with $\delta=0.549$. The best fit is for $\mu=2.2$. The solid line corresponds to the scaling distribution in Eq. (50) with $z(\delta)=1.36$ and the scale factor $c=0.36$. Although the fit is not too bad, it is actually somewhat inconsistent because $z(\delta)$ and μ should be related by Eq. (49), which would require $z=1.2$. However, this choice of $z(\delta)$ works less well.

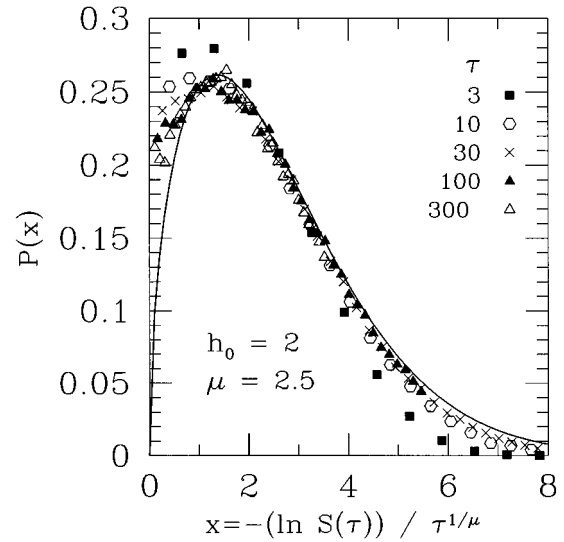


FIG. 10. As for Fig. 8 but with $\delta=0.346$. The best fit is for $\mu=2.5$. The solid line corresponds to the scaling distribution in Eq. (50) with $z(\delta)=2.0$ and the scale factor $c=0.46$. However, this is inconsistent since, according to the theory in the Appendix, μ and $z(\delta)$ should be related by Eq. (49), which would require $z=1.5$. However, this choice of $z(\delta)$ works less well.

shows that the *typical* correlation function, which we define to be the exponential of the average of the log, is given by

$$S_{\text{typ}}(\tau) \equiv \exp([\ln S(\tau)]_{\text{av}}) \sim \exp(-c\tau^{1/\mu}), \quad (52)$$

where c is a constant, i.e., a stretched exponential. This contrasts with the average, which varies as a power of τ , as shown in Eq. (46).

The average value is dominated by rare regions which have a much larger correlation function at long times than in a typical region. It is interesting to ask whether the average value is contained within the scaling function, or whether it comes from contributions which are actually corrections to scaling. We shall argue that there are *both* scaling and non-scaling contributions to the $\tau^{1/z(\delta)}$ behavior in Eq. (46). Similar behavior has been found recently for the distribution of the equal-time end-to-end correlation function at the critical point.²⁴

To estimate the contribution from the scaling function, we assume that the distribution, $P(x)$, of the scaling variable x , in Eq. (48), has the form x^a in the limit $x \rightarrow 0$, the only region which contributes to the average. This is indeed the case for the phenomenological theory discussed in the Appendix, for which $P(x)$ is given in Eq. (50). Since $S(\tau) = \exp(-x\tau^{1/\mu})$, it follows that the scaling contribution to the average is

$$S_{\text{av}}(\tau) \sim \int_0^\infty x^a \exp(-x\tau^{1/\mu}) dx \sim \frac{1}{\tau^{(1+a)/\mu}}, \quad (53)$$

which is of the form in Eq. (46) with the identification

$$z(\delta) = \frac{\mu}{1+a}. \quad (54)$$

Note that the phenomenological theory, Eqs. (49)–(51), satisfies this condition with

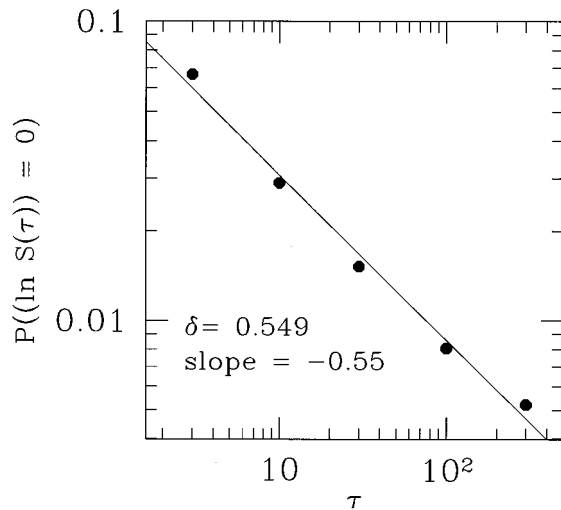


FIG. 11. The probability of $y = -\ln S(\tau)$ at $y=0$ for different values of τ for $\delta=0.549$ and $L=64$. The slope is -0.55 which is somewhat less than, but not too far from the value of $1/z(\delta)$ in Fig. 6. Hence this finite value of the probability at $\ln S(\tau)=0$ (which is a correction to the scaling form) gives a contribution to the power law decay of the average correlation function shown in Eq. (46).

$$a = \frac{1}{z(\delta)}. \quad (55)$$

Although the numerical data only fit the phenomenological theory close to the critical point with values of μ and $z(\delta)$ which are inconsistent with Eq. (49), this may be due to the times studied not being long enough and other corrections to scaling. It seems very likely that there *is* a contribution to the average time dependent correlation function from the scaling function.

However, we shall now argue that there is an additional contribution to the average correlation function, which comes from *corrections* to scaling. The exponent a is positive, so $P(0)=0$ in the scaling limit. However, we see from the data in Fig. 7 that the value of $\text{Prob}[-\ln S(\tau)=0]$ is finite for finite τ though it does decrease for large τ . This finite intercept is a correction to scaling. It is easy to see that if $\text{Prob}[-\ln S(\tau)=0] \sim \tau^{-1/z(\delta)}$, then this finite intercept will give a power law contribution to the average correlation function of the form in Eq. (46). Results for $\text{Prob}[-\ln S(\tau)=0]$ for different values of τ at $\delta=0.549$ are shown in Fig. 11. The slope is -0.55 , which is a little less than the estimate for $1/z(\delta)$ obtained by other methods, see Fig. 6, but since there are errors in extrapolating the data to $S(\tau)=0$, this is perhaps not significant. Hence our results suggest that $\text{Prob}[-\ln S(\tau)=0]$ vanishes as $\tau^{-1/z(\delta)}$, which gives an additional contribution to the average correlation function which is not contained within the scaling function.

VI. CONCLUSIONS

We have studied the paramagnetic phase of the disordered one-dimensional Ising chain in a transverse field. *Average* properties (equal time, time dependent, and temperature dependent) can be characterized by a continuously varying exponent $z(\delta)$. At criticality, $z(0)=\infty$ and, for the model studied, $\lim_{\delta \rightarrow \infty} z(\delta)=1$. As an example, the average, on-site,

time dependent correlation function decays with a continuously varying exponent, see Eq. (46). There are some discrepancies between the values of $z(\delta)$ obtained in different ways. We suspect that they are due to corrections to scaling, but one should perhaps also worry that the simple phenomenological picture in Sec. IV may be inadequate.

By contrast, the *typical* time dependent correlation function decays with the stretched exponential form in Eq. (52), where the exponent μ is probably given by Eq. (49), though our data close to the critical point shows some discrepancy with this. At long times, the distribution of $S(\tau)$ has a scaling form, being a function, $P(x)$, of the single variable x in Eq. (48). This may be given by Eq. (50), though corrections to scaling in the small x region prevent us from checking this thoroughly. For example, the data in the scaling plots in Figs. 8–10 are expected to go through the origin, but they actually do not, the discrepancy being larger for smaller τ .

The average of $S(\tau)$ arises both from the small x region of the scaling function, and from corrections to scaling.

It is interesting to ask to what extent the behavior in the paramagnetic phase is universal. Presumably the dependence of z on δ is nonuniversal (except close to the critical point⁴) but, for a given z , is the scaling function for the distribution of local correlation functions universal? Since the scaling function involves the limit of long times, it is possible that the microscopic details do not matter, only the form of the low energy density of states, in which case the distribution would be universal.

It would be interesting to see to what extent the results found here in one dimension go over to higher dimensions.

ACKNOWLEDGMENTS

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APPENDIX

Following the suggestion of Fisher,²³ we assume a simple phenomenological picture in which there are cluster excitations localized about different sites. It is plausible that the wave function of an excitation will decay exponentially with a distance of order the typical correlation function, ξ_{typ} . The contribution to the dynamics of site at the origin from an excitation centered n lattice spacings away will therefore be $\exp(-r/\xi_{\text{typ}} - \epsilon_n \tau)$. The local correlation function is therefore given by

$$S(\tau) = A \sum_{n=0}^{\infty} \exp\left(-\frac{r}{\xi_{\text{typ}}} - \epsilon_n \tau\right), \quad (A1)$$

where

$$A = 1 - e^{1/\xi} \quad (\approx \xi^{-1} \quad \text{for } \xi \gg 1) \quad (A2)$$

ensures that $S(0)=1$.

As a simple model we will assume that the ϵ_n are uncorrelated. Writing $\epsilon_n = \epsilon_0 e_n$, where ϵ_0 is a characteristic energy scale, we take the distribution of the e_n to be

$$\rho(e) = (\lambda + 1)e^\lambda \quad (0 < e < 1), \quad (\text{A3})$$

where we see from Eq. (41) that

$$\lambda = \frac{1}{z(\delta)} - 1. \quad (\text{A4})$$

Note that at large τ there is a competition between the $\exp(-r/\xi_{\text{typ}})$ factor in Eq. (A1), which decreases with increasing r and so would prefer to have r small, and the $\exp(-\epsilon_n \tau)$ factor which wants to have the smallest ϵ_n , which may be on a site far away.

The average value is easy to work out, since each term in Eq. (A1) can be evaluated separately, with the result

$$[S(\tau)]_{\text{av}} = \frac{\Gamma(1 + 1/z)}{(\epsilon_0 \tau)^{1/z}}, \quad (\text{A5})$$

for $\tau \gg 1$, where we used Eq. (A4).

However, the average is very different from the typical behavior. To see this, we will determine the full distribution of $S(\tau)$. The major simplification in the calculation is that, at large times, the exponent in Eq. (A1) varies over a large range, so the sum will be dominated by the largest single term. Writing Eq. (A1) as

$$S(\tau) = A \sum_{n=0}^{\infty} \exp\left(-\frac{x_n}{\xi_{\text{typ}}}\right), \quad (\text{A6})$$

where

$$x_n = n + \xi_{\text{typ}} \epsilon_0 \tau e_n, \quad (\text{A7})$$

then $S(\tau)$ is given for large τ by

$$S(\tau) \approx A \exp\left(\frac{-x_{\min}}{\xi_{\text{typ}}}\right), \quad (\text{A8})$$

where x_{\min} is the smallest of the x_n .

For the time being we will work in units of time where $\xi_{\text{typ}} \epsilon_0 = 1$. At the end, we will put back this factor by replacing τ by $\xi_{\text{typ}} \epsilon_0 \tau$.

The probability of x_n is given by

$$\pi_n(x_n) = \frac{\lambda + 1}{\tau} \left(\frac{x_n - n}{\tau}\right)^\lambda, \quad (\text{A9})$$

for $n < x_n < n + \tau$ and zero otherwise. Notice that the different x_n have different distributions.

We now wish to determine the probability that minimum value of the x_n is x_{\min} . Let us assume first that it is x_m which has the smallest value. The probability that (i) x_m is the smallest and (ii) its value is x_{\min} is given by

$$\frac{\pi_n(x_{\min})}{Q_n(x_{\min})} \prod_{n=0}^{\infty} Q_n(x_{\min}), \quad (\text{A10})$$

where

$$Q_n(x_{\min}) = \int_{x_{\min}}^{n+\tau} \pi_n(x) dx. \quad (\text{A11})$$

Since $\pi_n(x)$ vanishes for $x < n$, it follows that for $n > x_{\min}$, the full range over which $\pi_n(x)$ is nonzero is included in the last integral, and so

$$Q_n(x_{\min}) = 1 \quad (n > x_{\min}). \quad (\text{A12})$$

As a result, the product in Eq. (A10) need only be taken up to the last integer below x_{\min} . For $n < x_{\min}$, one has

$$Q_n(x_{\min}) = 1 - \left(\frac{x_{\min} - n}{\tau}\right)^{\lambda+1}. \quad (\text{A13})$$

We will see that $x_{\min} \ll \tau$ and the important values of m are those where $1 \ll m \ll \tau$, and so we can rewrite Eq. (A10) as

$$\frac{\lambda + 1}{\tau} \left(\frac{x_{\min} - m}{\tau}\right)^\lambda \exp\left\{\int_0^{x_{\min}} \ln\left[1 - \left(\frac{x_{\min} - x}{\tau}\right)^{\lambda+1}\right] dx\right\}. \quad (\text{A14})$$

Expanding the log using $x_{\min} - x \ll \tau$ and performing the integral gives

$$\frac{\lambda + 1}{\tau} \left(\frac{x_{\min} - m}{\tau}\right)^\lambda \exp\left[-\frac{x_{\min}^{\lambda+2}}{(\lambda + 2)\tau^{\lambda+1}}\right]. \quad (\text{A15})$$

Remember that this is the probability that x_m is the smallest of the x_n and its value if x_{\min} . We therefore next sum over all m less than x_{\min} to get the total probability that the minimum is x_{\min} , i.e.,

$$P_{\min}(x_{\min}) = \left(\frac{x_{\min}}{\tau}\right)^{\lambda+1} \exp\left[-\frac{x_{\min}^{\lambda+2}}{(\lambda + 2)\tau^{\lambda+1}}\right]. \quad (\text{A16})$$

Replacing τ by $\epsilon_0 \xi_{\text{typ}} \tau$, and changing variables from x_{\min} to $y \equiv -\ln[S(\tau)/A]$ using Eq. (A8), gives

$$P_y(y) = \xi_{\text{typ}} \left(\frac{y}{\epsilon_0 \tau}\right)^{\lambda+1} \exp\left[-\frac{\xi_{\text{typ}} y^{\lambda+2}}{\lambda + 1 (\epsilon_0 \tau)^{\lambda+1}}\right]. \quad (\text{A17})$$

It is easy to check that this yields the average value in Eq. (A5).

Equation (A17) can be cast in a scaling form if we define

$$x = \frac{y}{\tau^{1/\lambda}} = -\frac{\ln(S(\tau)/A)}{\tau^{1/\lambda}}. \quad (\text{A18})$$

Note, however, that the scaling limit involves taking $-\ln S(\tau) \rightarrow \infty$ so the $\ln A$ term in Eq. (A18) represents an additive *correction* to scaling and can be omitted. This then leads to Eq. (51), in which λ has been replaced by z using Eq. (A4). The probability of x is then a function just of x (apart from a scale factor), i.e.,

$$P(x) = c(cx)^{1/z} \exp\left[-\frac{z}{z+1}(cx)^{(z+1)/z}\right], \quad (\text{A19})$$

where we have again expressed the result in terms of z rather than λ using Eq. (A4), and

$$c = (\xi_{\text{typ}}^z \epsilon_0)^{1/(z+1)}. \quad (\text{A20})$$

Equation (A20) is precisely Eq. (50) of the text.

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- ¹⁶Note that ϵ_μ , as defined here, corresponds to $2\epsilon_\mu$ in YR. With our present definition, ϵ_μ is the energy of a Fermi excitation; see Eq. (13), which seems to be the most natural notation.
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