Density Profiles in Random Quantum Spin Chains

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We consider random transverse-field Ising spin chains and study the magnetization and the energy-density profiles by numerically exact calculations in rather large finite systems ($L \leq 128$). Using different boundary conditions (free, fixed, and mixed) the numerical data collapse to scaling functions, which are very accurately described by simple analytic expressions. The average magnetization profiles satisfy the Fisher–de Gennes scaling conjecture and the corresponding scaling functions are indistinguishable from those predicted by conformal invariance. [S0031-9007(97)02733-6]

Every experimental system is geometrically constrained and therefore has a surface, for which reason we have to discriminate between so-called *bulk* and *surface* properties. This is justified as long as the correlation length is much smaller than the system size. However, *at* a critical point it is more appropriate to describe the position dependent physical properties of the system by density profiles rather than bulk and/or surface observables. For a number of universality classes much is known about this spatially inhomogeneous behavior [1], in particular in two dimensions, where conformal invariance provides a powerful tool to study various geometries [2].

Not much is known about this issue for quantum systems with quenched (i.e., time independent) *disorder*. Here one is confronted with a possible quantum phase transition, i.e., a zero temperature transition that is triggered by quantum rather than thermal fluctuations, as for instance in random transverse field Ising models [3–5]. Their bulk properties have been studied quite extensively by now. The aim of the present Letter is to investigate for the first time the above mentioned density profiles in a geometrically constrained disordered system at a quantum phase transition. In particular we study numerically the random transverse field Ising chain and propose analytic expressions of the magnetization and energy-density profile for various boundary conditions (b.c.).

In a critical system confined between two parallel plates, being a large but finite distance L apart, the local densities $\langle \Phi(r) \rangle$ such as the order parameter (magnetization) or the energy density vary with the distance l from one of the plates as a smooth function of l/L. According to the scaling theory by Fisher and de Gennes [6],

$$\langle \Phi(l) \rangle_{ab} = L^{-x_\Phi} F_{ab}(l/L), \quad (1)$$

where x_Φ is the scaling dimension of the operator Φ, while ab denotes the b.c. at the two plates. The scaling function in (1) has the asymptotic behavior

$$F_{ab}(l/L) = A\left[1 + B_{ab}\left(\frac{l}{L}\right)^d + \dot{s} \right]; \quad \frac{l}{L} \ll 1, \quad (2)$$

where the exponent in the first correction term was confirmed by different methods [7–9]. It has been shown by Burkhardt and Xue [10] and by Cardy [9] that the B_{ab} coefficients in (2) and the A_{ab} finite-size correction coefficients of the free energy as $A_{ab}L^{-d+1}$ are related to each other: Their ratio is universal and independent of the form of the b.c.

Having the same type of b.c. at both plates the profile $\langle \Phi(l) \rangle_{aa} = L^{-x_\Phi} f_{aa}(l/L)$ is reflection symmetric $f_{aa}(v) = f_{aa}(1 - v)$ and according to Eqs. (1) and (2) $\lim_{v \to 0} f_{aa}(v) \sim v^{-x_\Phi}$. Consequently, $[f_{aa}(v)]^{-1/x_\Phi}$ can be expanded in a Fourier series [11], which yields

$$\langle \Phi(l) \rangle_{aa} = L^{-x_\Phi}\left[\sum_{k=1}^{\infty} A_k \sin\frac{k\pi l}{L} \right]^{-x_\Phi}. \quad (3)$$

The Fourier expansion in (3) has different convergence properties in two and three dimensions due to the different parity of the correction term in (2). While in three dimensions infinite terms are needed to reproduce the Fisher–de Gennes scaling result in (2), in two dimensions one expects to obtain satisfactory accuracy by the first few terms of the expansion. Indeed for conformally invariant two-dimensional models only the first term in the Fourier series in (3) gives nonvanishing contribution [8]:

$$\langle \Phi(l) \rangle_{aa} = A\left[\frac{L}{\pi}\sin\pi\frac{l}{L} \right]^{-x_\Phi}. \quad (4)$$

Conformal invariance can be used further to predict the density profiles with general b.c. In two dimensions the profiles are in the form [10]

$$\langle \Phi(l) \rangle_{ab} = \left[\frac{L}{\pi}\sin\pi\frac{l}{L} \right]^{-x_\Phi} G_{ab}\left(\frac{l}{L}\right), \quad (5)$$

where the scaling function $G_{ab}(l/L)$ depends on the universality class of the model and on the type of the b.c.

For the Ising model the magnetization profile with free-fixed b.c. the scaling function is predicted as [10]

$$G_{f+} = B\left[\sin\frac{\pi l}{2L}\right]^{x_m^s},\tag{6}$$

where $x_m^s = 1/2$ is the scaling dimension of the surface magnetization operator. A similar result is obtained for the $Q \leq 4$ state Potts model [10] with the appropriate surface scaling dimension in (6).

In the present Letter we consider the random transverse field Ising chain

$$\hat{H} = -\sum_l J_l \sigma_l^x \sigma_{l+1}^x - \sum_l h_l \sigma_l^z.\tag{7}$$

Here the J_l exchange couplings and the h_l transverse fields are independent random variables with distributions $\pi(J)$ and $\rho(h)$, respectively, and the σ_l^x, σ_l^z are Pauli matrices at site l. This Hamiltonian is the extreme anisotropic limit [12] of the layered two-dimensional Ising model as introduced by McCoy and Wu [13,14].

The critical behavior of the random transverse-field Ising spin chain in (7) has been investigated analytically [3,14,15] and numerically [16,17] in several papers. Depending on the strength of the average value of the transverse field the system has two phases, which are separated by a second order phase transition point located at [15] $\delta = \overline{\ln J} - \overline{\ln h} = 0$. Because of a broad distribution of various physical quantities the typical and average quantities of the system are generally different. The scaling dimensions of the averaged magnetization are $x_m = (3 - \sqrt{5})/4 \approx 0.191$ [3] and $x_m^s = 1/2$ [14]. The model is anisotropic at the critical point; the dynamical exponent is $z = \infty$. More precisely the characteristic length scale ξ and the corresponding time scale t are related through

$$\ln t \sim \sqrt{\xi}.\tag{8}$$

Thus the model is not conformally invariant and predictions in Eqs. (4)–(6) are not expected to be valid.

In the following we briefly describe how the density profiles were calculated. For *fixed* boundary conditions, which break the up-down symmetry of the Hamiltonian in Eq. (7), the local magnetization defined as

$$m(l) = \langle 0|\sigma_l^x|0\rangle\tag{9}$$

is finite for any finite system. On the other hand, for *free* (nonsymmetry breaking) b.c. the magnetization in a finite system is zero, due to symmetry. In this case one considers the asymptotic behavior of the (imaginary) time-time correlation function $G_l(\tau) = \langle \sigma_l^x(\tau)\sigma_l^x(0)\rangle = \sum_i |\langle i|\sigma_l^x|0\rangle|^2 \exp[-\tau(E_i - E_0)]$ where $\langle 0|$ and $\langle i|$ denote the ground state and the ith excited state with energies E_0 and E_i, respectively. In the large τ limit the sum is dominated by the first term, and the corresponding off-diagonal (o.d.) matrix element

$$\sigma_{\text{od}}(l) = \langle 1|\sigma_l^x|0\rangle\tag{10}$$

is of interest. In the strong coupling phase ($\delta < 0$), where E_1 is asymptotically degenerate with the ground state,

in the thermodynamic limit $m(l) = \sigma_{\text{od}}(l)$. In a finite system bulk and surface magnetization exponents can be deduced from the o.d. matrix element in Eq. (10) [2].

The energy-density profile is given by the ground state expectation value $e(l) = \langle 0|\sigma_l^z|0\rangle$. Since $e(l)$ contains a nonsingular contribution the scaling behavior of the energy density is more convenient to deduce from the asymptotic form of the connected time-time correlation function $G_l^e(\tau) = \langle \sigma_l^z(\tau)\sigma_l^z(0)\rangle - \langle \sigma_l^z(\tau)\rangle\langle \sigma_l^z(0)\rangle = \sum_i \times |\langle i|\sigma_l^z|0\rangle|^2 \exp[-\tau(E_i - E_0)]$ of the energy-density operator σ_l^z. Then, similarly to the order parameter the singular energy density $\epsilon(l)$ is given by

$$\epsilon(l) = \langle \epsilon|\sigma_l^z|0\rangle,\tag{11}$$

where $\langle \epsilon|$ denotes the lowest excited state that yields a nonvanishing matrix element $\langle \epsilon|\sigma_l^z|0\rangle$. This o.d. matrix element is of interest in the finite-size scaling study of the bulk and surface energy-density operators [18].

To calculate the matrix elements in Eqs. (9)–(11), we first, following Lieb *et al.* [19] and Pfeuty [20], transform $\hat{H}$ into a free-fermion model. For the fixed and free b.c. we study in this Letter we found it most convenient to choose the representation described in [21], which necessitates only the diagonalization of an $2L \times 2L$-tridiagonal matrix. From the corresponding eigenvectors one obtains the local magnetization (9) and the matrix elements (10) and (11) [22]. Details will be presented elsewhere [23].

The critical properties of random Ising chains are expected to be independent of the details of the distributions of the couplings and/or fields. In this Letter we consider two different cases: the binary distribution

$$\pi(J) = \frac{1}{2}\,\delta(J - \lambda) + \frac{1}{2}\,\delta(J - \lambda^{-1}); \qquad h = h_0,\tag{12}$$

i.e., $\rho(h) = \delta(h - h_0)$, and the uniform distribution

$$\pi(J) = \theta(1 - J)\theta(J); \qquad \rho(h) = h_0^{-1}\theta(h_0 - h)\theta(h).\tag{13}$$

In both cases the critical point is at $h_0 = 1$. All numerical data which we present below are averaged over 50 000 samples and the resulting statistical error is much smaller than the size of the symbols used in the plots. Disorder-averaged quantities are denoted by the brackets $[\cdots]_{\text{av}}$.

First we study the magnetization profile of the system with fixed b.c. at both ends of the chain. The finite-size results on the pure model, which are shown in the inset of Fig. 1, are in complete agreement with the conformal prediction in (4). The profile for the random chain is shown in Fig. 1. From the scaling plot one can see that the Fisher–de Gennes scaling result in (1) is well satisfied with the conjectured value of the decay exponent $x_m = \beta/\nu = 0.191$. Note that we do *not* use x_m (as well as later x_m^s) as fit parameters but fix them to the theoretically predicted values cited above. The only fit parameter is the nonuniversal prefactor A in (4). Obviously, one can
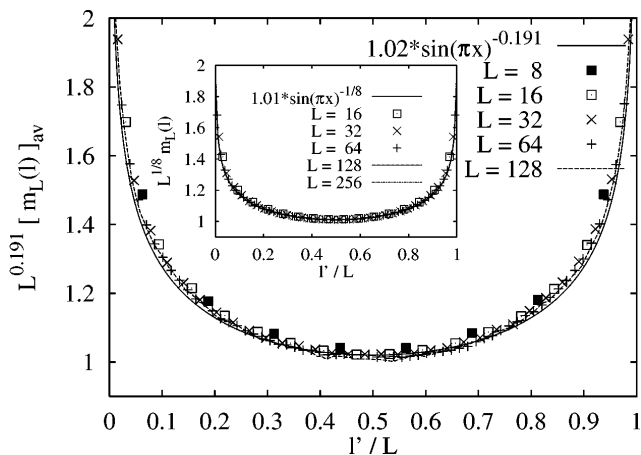
FIG. 1. Scaling plot of the magnetization profile $m_L(l)$ (9) with fixed b.c. at both ends. We have shifted the site index by half a lattice constant and denote $l' = l - 0.5$. The pure case is depicted in the inset, for which the scaling function is given by (5) with $x_m^{pure} = 1/8$ and $G_{++} = $ const. The main figure shows the result for the binary distribution (12) with $\lambda = 4$. Other values of λ as well as the uniform distribution yield the same quality for the data collapse, with different values for the nonuniversal prefactors but identical scaling function (5) with $x_m^{random} = \beta/\nu \approx 0.191$ and $G_{++} = $ const.

very accurately describe the finite-size data in the whole profile with the first term of the Fourier expansion in (3). The corrections to the conformal result in (4) are indeed negligible.

Next we turn to study the magnetization profiles with free-fixed b.c. As seen on the inset of Fig. 2 the finite-lattice results on the pure model perfectly coincide with the conformal prediction in (6). Results for random models are shown in Fig. 2. As one can see the numerical data collapse to a scaling function, which can be very
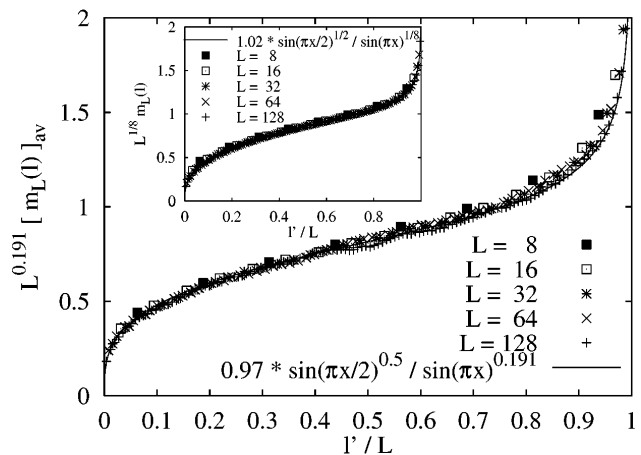
accurately described by a function of the form in (6) with the exponents $x_m = 0.191$ and $x_m^s = \beta^s/\nu = 1/2$ [again the only fit parameter is the nonuniversal prefactor B from (6)]. According to Fig. 2 the corrections to the conformal result seem here also to be negligible.

With free (nonsymmetry breaking) b.c. the magnetization is zero in a finite system. Therefore we consider the o.d. density in Eq. (10), the profile of which can be predicted by conformal invariance [18]. For a general local operator $\hat{\Phi}(l)$ the scaling form of the o.d. matrix element in the strip geometry is [18]

$$\langle 0|\hat{\Phi}(l)|\Phi\rangle \propto \left(\frac{\pi}{L}\right)^{x_\Phi}\left(\sin\pi\frac{l}{L}\right)^{x_\Phi^s - x_\Phi}, \quad (14)$$

where x_Φ^s denotes the surface scaling dimension of $\hat{\Phi}$. This expression satisfies the known scaling limits $\langle 0|\hat{\Phi}(1)|\Phi\rangle \sim L^{-x_\Phi^s}$ and $\langle 0|\hat{\Phi}(L/2)|\Phi\rangle \sim L^{-x_\Phi}$ at the surface and in the bulk, respectively. For nonconformally invariant systems (14) represents the first leading term of a Fourier-expansion, as in (3) and (4).

Numerical results on the o.d. density profiles with free b.c. are shown on Fig. 3. Again the finite-size results on the pure Ising model are in complete coincidence with the conformal prediction in (14). For the random case the numerical data collapse to a scaling curve, which is very accurately described by the conformal expression in (14) with the exponents $x_m = 0.191$ and $x_m^s = 1/2$. Thus again the nonconformal corrections are very small.

Finally, we discuss the o.d. energy-density profile in (11). For the pure model one can easily evaluate $\epsilon(l)$, which yields in the scaling limit ($l \gg 1, L \gg 1$)

$$\epsilon(l) = \frac{2}{L}\sin\pi\frac{l}{L}. \quad (15)$$

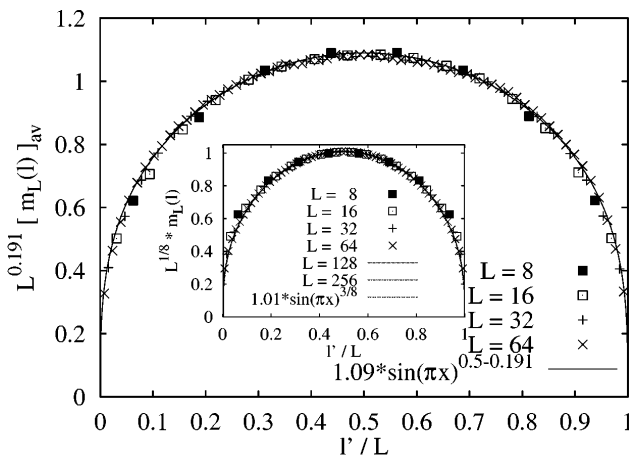See inset of Fig. 4. This corresponds to the conformal result in Eq. (14) with $x_e = 1$ and $x_e^s = 2$.

FIG. 2. The same as in Fig. 1 with fixed b.c. on the right end of the chain and free b.c. on the left end. The magnetization profile is given by (5) and (6) with $x_m^s = 1/2$ for the pure *and* the random case. The data shown in the main figure are for the uniform distribution (13).

FIG. 3. Scaling plot of the o.d. magnetization profile $\sigma_{od}(l)$ [Eq. (10)] for free b.c. on both ends of the chain. The data for the random case are for a binary distribution with $\lambda = 2$. The full line represents the scaling form (14).
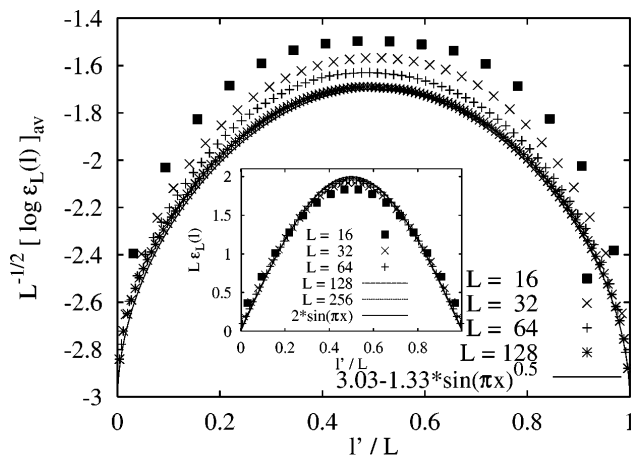
FIG. 4. The o.d. energy profile $\epsilon_L(l)$ (11) with free b.c. on both sides. The pure case is depicted in the inset, for which the scaling function is given by (15). The main figure shows the result for the binary distribution (12) with $\lambda = 4$. Here the scaling function is well described by (16). We note that the approach to the asymptotic scaling limit seems to be much slower than for the magnetization profiles.

In a quantum system the bulk energy density is proportional to the inverse relaxation time: $\epsilon \sim t^{-1}$. In the random transverse Ising chain the scaling is anomalous as indicated in (8), therefore the appropriate scaling combination is $L^{-1/2}\ln\epsilon(l)$ instead of $L\epsilon(l)^{1/z}$ if z would be finite. In the following we study the typical energy density $[\ln\epsilon(l)]_{\mathrm{av}}$, which after multiplication with $L^{-1/2}$ yields a universal scaling function. The finite-size data for the random case (see Fig. 4) very well satisfy the relation

$$[\ln\epsilon(l)]_{\mathrm{av}} L^{1/2} = A_0 + A_1\left(\frac{L}{\pi}\sin\pi\frac{l}{L}\right)^{1/2}. \qquad (16)$$

We note that this expression can also be considered as the leading part of a Fourier expansion, where the correction terms are again very small.

To summarize we have investigated the density profiles of random transverse-field Ising spin chains. The numerical data on rather large systems $L \leq 128$ follow scaling plots and the scaling functions can be described very accurately by analytical expressions, which are derived for conformally invariant systems. Since our system is not conformally invariant there are presumably corrections. These are, however, very small, certainly smaller than the error in our present numerical calculation.

Generally the nonconformal corrections to the density profiles are not small. As an example, we mention the two-dimensional aperiodically layered Ising model [24], which is somewhat related to our problem. When the aperiodically modulated couplings of the model represent a marginal perturbation the system is described by a coupling dependent dynamical exponent $z > 1$ [21], thus the system is not conformally invariant. Although the aperiodic model looks similar to our random problem its density pro-

files are completely different from the conformal results [22]. One could speculate about the existence of some hidden symmetry which explains the coincidence of the density profiles of the random transverse-field Ising chain with the conformal result.

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