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.

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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, in particular in two dimensions, where conformal invariance provides a powerful tool to study various geometries.

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 Ising models. 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, which are a large but finite distance $L$ apart, the local densities $\langle \Phi(l) \rangle_{ab}$ 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:

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

where $x_{ab}$ is the scaling dimension of the operator $\Phi$, while $ab$ denotes the boundary conditions at the two plates. The scaling function in (1) has the asymptotic behavior:

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

where the exponent in the first correction term was confirmed by different methods. It has been shown by Burkhardt and Xue and by Cardy 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 $\langle \Phi(l) \rangle_{aa} = L^{-\gi_{aa}} f_{aa}(l/L)$ is reflection symmetric $f_{aa}(v) = f_{aa}(1-v)$ and according to eqs. (1) and (4) $\lim_{v \to 0} f_{aa}(v) \sim v^{-x_{ab}}$. Consequently $[f_{aa}(v)]^{-1/x_{ab}}$ can be expanded in a Fourier series and the profile is given by:

$$\langle \Phi(l) \rangle_{aa} = L^{-x_{ab}} \left[ \sum_{k=1}^{\infty} A_k \sin \frac{k \pi l}{L} \right]^{-x_{ab}}$$  (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 (3), in two-dimensions one expect 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 non-vanishing contribution.

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

$$\langle \Phi(l) \rangle_{ab} = \left[ \frac{L}{\sin \frac{\pi l}{L}} \right]^{-x_{ab}} G_{ab} \left( \frac{l}{L} \right)$$  (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 boundary condition the scaling function is predicted as
\[ G_f = B \left[ \sin \left( \frac{\pi l}{2L} \right) \right]^{x_m} \]  
where \( x_m = 1/2 \) is the scaling dimension of the surface magnetization operator. Similar result is obtained for the \( Q \leq 4 \) state Potts model with the appropriate surface scaling dimension in [15].

In the present Letter we consider the random transverse filed Ising chain
\[ \hat{H} = -\sum_l J_l \sigma^z_l \sigma^z_{l+1} - \sum_l h_l \sigma^x_l \]  
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 \( \sigma^x_l, \sigma^z_l \) are Pauli matrices at site \( l \). This Hamiltonian is the extreme anisotropic limit of the layered two-dimensional Ising model as introduced by McCoy and Wu.

The critical behavior of the random transverse-field Ising chain in [16] has been investigated analytically [16,17] and numerically 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 
\[ \begin{align*} 
\delta &= \ln J - \ln h = 0. 
\end{align*} \]
Due to 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 
\[ x_m = (3 - \sqrt{5})/4 \approx 0.191 \]  
and \( x_m = 1/2 \) [18,19]. The model is anisotropic at the critical point, the dynamical exponent is \( z = \infty \). More precisely the characteristic length scale \( \xi \) and the corresponding time scale \( t \) are related through:
\[ \ln t \sim \sqrt{\xi} \]  
thus the model is not conformally invariant and predictions in eqs. (6) are not expected to be valid.

In the following we briefly describe how the density profiles were calculated. The local magnetization \( m_l \) is obtained from the asymptotic behavior of the (imaginary) time-time correlation function \( G_l(\tau) = \langle \sigma^z_l(\tau) \sigma^z_l(0) \rangle = \sum_i |\langle i | \sigma^z_l | 0 \rangle|^2 \exp(-\tau(E_i - E_0)) \) where \( |0\rangle \) denote the ground state and the \( i \)-th excited state with energies \( E_0 \) and \( E_i \), respectively. In the low temperature (strong coupling) phase \( E_1 \) is asymptotically degenerate with the ground state, thus the sum is dominated by the first term. In the large \( \tau \) limit \( G_l(\tau) = m_l^2 \), therefore the local magnetization is given by
\[ m_l = \langle 1 | \sigma^z_l | 0 \rangle \]  
The energy-density profile is given by the ground state expectation value \( \epsilon_l = \langle 0 | \sigma^z_l | 0 \rangle \). Since \( \epsilon_l \) contains a non-singular contribution the scaling behavior of the energy-density is more convenient to deduce from the asymptotic form of the connected time-time correlation function of the energy-density operator \( \sigma^z_l \). Similarly to the order-parameter the singular energy density \( \epsilon_l \) is given by a matrix-element:
\[ \epsilon_l = \langle \epsilon | \sigma^z_l | 0 \rangle \]  
where \( \langle \epsilon \rangle \) denotes the first excited state, which has non-vanishing matrix-element with the ground state.

To calculate the matrix-elements in eqs. (4,10) we first, following Lieb et al. and Pfeuty transform \( H \) 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 [18], which necessitates only the diagonalization of an \( 2L \times 2L \)-tridiagonal matrix. From the corresponding eigenvectors one obtains the local magnetization \( \epsilon \) and local energy density \( \epsilon \) as described in [16].

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
\[ \pi(J) = \frac{1}{2} \delta(J - \lambda) + \frac{1}{2} \delta(J - \lambda^{-1}) \quad h = h_0 , \]  
i.e. \( \rho(h) = \delta(h - h_0) \), and the uniform distribution:
\[ \pi(J) = \theta(1 - J) \theta(J) \quad \rho(h) = \theta(h_0 - h) \theta(h) \]
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 \([\ldots]\).

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 [16]. 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 [16] 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 \( x_m \)) as fit parameters but fix them to the theoretically predicted values cited above. The only fit parameter is the non-universal prefactor \( A \) in [16]. Obviously, one can very accurately describe the finite-size data in the whole profile with the first term of the Fourier expansion in [16]. The corrections to the conformal result in [16] 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 [16]. 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 [16] with the exponents: \( x_m = 0.191 \) and \( x_m = \beta/\nu = 1/2 \) (again the
conformal result seems here also to be negligible.

From (4-5). According to Fig. 2 the corrections to the
A only fit-parameter is the non-universal prefactor
with \( x \) is depicted in the inset, for which the scaling function is given
by (5) with \( x \) is the random case. The data shown in the main figure are
for the uniform distribution (12).

Due to symmetry the magnetization in a finite system
with free (non-symmetry breaking) b.c. is zero. However,
introducing an infinitesimal symmetry breaking field \( h \)
one can obtain the magnetization by Yang’s method
with the identical result as in (1). Then, as \( h \to 0 \) the
matrix-element in (3) can be considered to define the
local magnetization in a finite system in a time scale
\( \tau \ll t \), where \( t \) is the relaxation time. The profile of
the matrix-element in (3) can be predicted by conformal
invariance (2). For a general local operator \( \hat{\Phi}(l) \) the scaling
form in the strip geometry is given by:

\[
\langle 0|\hat{\Phi}(l)|\Phi \rangle \propto \left( \frac{\pi}{L} \right)^{x_{\Phi}} \sin \left( \frac{\pi}{L} l \right)^{x_{\Phi}-x} \tag{13}
\]

where \( x_{\Phi} \) denotes the surface scaling dimension of \( \Phi \). This expression satisfies the known scaling limits
\( \langle 0|\hat{\Phi}(1)|\Phi \rangle \sim L^{-x_{\Phi}} \), and \( \langle 0|\hat{\Phi}(L/2)|\Phi \rangle \sim L^{-x_{\Phi}} \) at the
surface and in the bulk, respectively. For non-conformally
invariant systems (13) represents the first leading term
of a Fourier-expansion, as in (3) and (4).

Numerical results on the magnetization profiles with
free boundary conditions are shown on Fig. 3. Again the
finite-size results on the pure Ising model are in complete
coincidence with the conformal prediction in (13). For
the random case the numerical data collapse to a scaling
curve, which is very accurately described by the confor-
mal expression in (13) with the exponents \( x_m = .191 \) and
\( x_{\Phi} = 1/2 \). Thus again the non-conformal corrections are
very small.

Finally, we discuss the singular part of the energy den-
sity profile and study the energy density matrix-element
in (10). For the pure model one can easily evaluate \( \epsilon(l) \),
which yields in the scaling limit \( l \gg 1 \), \( L \gg 1 \):

\[
\epsilon(l) = \frac{2}{L} \sin \pi \frac{l}{L} \tag{14}
\]

This corresponds to the conformal result in eq.(13) with
\( x_e = 1 \) and \( x_{\Phi} = 2 \).

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

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

(15)

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 non-conformal corrections to the density profiles are not small. As an example we mention the two-dimensional aperiodically layered Ising model, 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 $z > 1$, thus the system is not conformally invariant. Although the aperiodic model looks similarly to our random problem its density profiles are completely different from the conformal result. 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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