Disorder induced cross-over effects at quantum critical points

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(March 22, 2022)

Critical properties of quantum spin chains with varying degrees of disorder are studied at zero temperature by analytical and extensive density matrix renormalization methods. Generally the phase diagram is found to contain three phases. The weak disorder regime, where the critical behavior is controlled by the fixed points of the pure system and the strong disorder regime, which is attracted by an infinite randomness fixed point, are separated by an intermediate disorder regime, where dynamical scaling is anisotropic and the static and dynamical exponents are disorder dependent.

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Quantum phase transitions take place at zero temperature due to quantum fluctuations by varying a quantum control parameter \(\nu\), which could be either the density of impurities (for the metal-insulator transition in three dimensions (3d) or for the superconducting-insulator transition in 2d) or an external thermodynamical parameter such as the strength of the magnetic field in quantum spin glasses or the pressure in BaVS\(_3\). The effect of quenched, i.e. time-independent disorder at quantum phase transitions is the subject of recent intensive research. We mention, for instance, the recent experimental studies about doping effects in quantum spin chains and ladders and a theoretical explanation about the non-Fermi liquid behavior in U and Ce intermetallics.

From a theoretical point of view several analytical and numerical studies have been performed mainly in low-dimensional systems. In particular in one dimension many, presumably exact, results have been obtained by the application of a strong disorder renormalization group (SDRG) method, originally introduced by Ma, Dasgupta and Hu. For the random transverse-field Ising model Fisher has shown that at the critical point the probability distributions of the couplings and the transverse fields broaden without limits under renormalization, and as a consequence the SDRG becomes asymptotically exact at the so-called infinite randomness fixed point (IRFP).

In the IRFP dynamical scaling is strongly anisotropic, such that the relaxation time, \(t_r\), and correlation length, \(\xi\), are related as: \(\ln t_r \sim \sqrt{\xi}\). Scaling of the static singular quantities can be conveniently described by the magnetization scaling dimensions, \(x\), (and similarly for surface spins by \(x^s\)) and by the critical exponent of the average correlation length, \(\nu\), which are given by

\begin{equation}
  x_{\text{IRFP}} = 3 - \frac{\sqrt{5}}{4}, \quad x_{\text{IRFP}}^s = \frac{1}{2}, \quad \nu_{\text{IRFP}} = 2.
\end{equation}

The asymptotically exact SDRG analysis of the random transverse-field Ising model has been extended into the off-critical region, i.e. into the Griffiths phase and the dynamical exponent, \(z\), connecting time- and length-scales as \(t_r \sim \xi^z\), has been analytically calculated.

The SDRG method has been applied for a series of random quantum systems at the transition point. Despite the fact, that in the absence of disorder, these systems have different type of (spatial and temporal) correlations, thus they are in different universality classes, the SDRG analysis indicates that if the disorder is strong enough all models are attracted by the IRFP of the random transverse-field Ising model. In that respect quantum fluctuations seem to be irrelevant, so that solely the strong disorder effects dominate the critical behavior.

However the SDRG approach does not provide any information on the behavior of the system at weak disorder. In this limit one generally invokes the Harris criterion according to which weak disorder is irrelevant if:

\begin{equation}
  \nu_0 > 2/d,
\end{equation}

where \(\nu_0\) is the correlation length critical exponent of the pure system. If \(\nu_0 < 2/d\), thus disorder is relevant the IRFP could be strongly attractive as for the random transverse-field Ising model, while if \(\nu_0 > 2/d\) only a finite amount of disorder may bring the system to the IRFP.

The aim of this Letter is to investigate in detail the weak to strong disorder crossover behavior at a quantum critical point and to present a possible common scenario. In view of the generality of this phenomenon and its possible relevance in realistic quantum systems it is of importance to perform a detailed study of the singular behavior of random quantum systems in the whole range of strength of disorder.

As a subject of our study we have chosen two one-dimensional quantum models, the q-state quantum clock
model (CM) and the quantum Ashkin-Teller (AT) model. Our selection is motivated by the following facts: i) both models are self-dual, thus the location of the critical point is exactly known. ii) The SDRG analysis can be performed for both models leading to IRFP behavior for strong disorder. iii) Critical properties of the pure models are given in details, in particular one can locate the part of the phase diagram, where the Harris irrelevance criterion is valid in the form of Eq. (3).

We start to introduce the quantum CM [20], which is defined by the Hamiltonian:

\[ H_{CM} = -\sum_{l} \left[ J_{l} \cos \frac{2\pi(s_{l} - s_{l+1})}{q} + \frac{\hbar_{l}}{2} \left( M_{l}^{x} + M_{l}^{y} \right) \right] , \]

in terms of a discrete spin variable, \( s_{l} = 1, 2, \ldots, q \), at a lattice site, \( l \), and \( M_{l}^{z} | s_{l} \rangle = | s_{l} \pm 1, \text{mod} q \rangle \) is a spin raising (lowering) operator.

Similarly the quantum AT model is defined by the Hamiltonian [21]:

\[ H_{AT} = -\sum_{l} J_{l} (\sigma_{l}^{x} \sigma_{l+1}^{x} + \tau_{l}^{z} \tau_{l+1}^{z}) - \epsilon \sum_{l} (J_{l} \sigma_{l}^{x} \tau_{l}^{z} + h_{l} \sigma_{l}^{x} \tau_{l}^{x}) , \]

in terms of two sets of Pauli matrices, \( \sigma_{i}^{x,z}, \tau_{i}^{x,z} \). For both models the couplings, \( J_{l} \), and the transverse fields, \( h_{l} \), are independent random variables, while for the AT model the coupling between the two Ising models, \( \epsilon \), is disorder independent. Both models are self-dual, which amounts to the invariance of the Hamiltonians in Eqs. (3) and (4) under the transformation \( J_{l} \leftrightarrow h_{l} \).

The pure CM, with \( J_{l} = J \) and \( h_{l} = h \), for \( q > 4 \) has an extended critical phase at both sides of the self-duality point, which is located at \( J = h \). According to our numerical results, obtained by the density matrix renormalization group (DMRG) method [22] the critical exponents of the \( q = 5 \) model at the self-duality point are given by:

\[ x_{CM} = 0.105(5), \quad x_{CM}^{x} = 0.23(1). \]

Since the self-duality point is located in the middle of a critical phase \( \nu_{CM} \) is formally infinity, thus small disorder is irrelevant, according to Eq. (3).

The pure quantum AT model is critical along the self-duality line for \(-1 < \epsilon < 0\) with the critical exponents:

\[ x_{AT} = \frac{1}{8}, \quad x_{AT}^{x} = \frac{\arccos(-\epsilon)}{\pi}, \quad \nu_{AT} = \frac{2x_{AT}^{x}}{4x_{AT} - 1} , \]

which are conjecturedly exact [21, 23]. For \(-1/\sqrt{2} < \epsilon < -1/2\) the correlation length exponent of the pure model, \( \nu_{AT} \), exceeds the value of 2, thus the Harris irrelevance criterion in Eq. (3) sets in. (We note that \( \nu_{AT} \) stays formally infinite in the whole region of \(-1 < \epsilon < -1/\sqrt{2}\), which is the central part of the so called critical fan [21].)

The SDRG transformation can be performed for both models leading to similar decimation rules:

\[ \tilde{h}_{i} = \frac{h_{i} h_{i+1}}{J_{i} \kappa}, \quad \tilde{J}_{i} = \frac{J_{i} J_{i+1}}{h_{i} \kappa} , \]

where the first (second) equation refers to the elimination of a strong bond (field) of strength, \( J_{i} \) (\( h_{i} \)). For the CM \( \kappa = [1 - \cos(2\pi/q)]/[1 + \delta_{2,q}] \) [13] and \( q \) does not renormalize under the transformation. On the other hand for the AT model, where, \( \kappa = 1 + \epsilon \), the coupling, \( \epsilon \), enters into the renormalization as \( \epsilon = \epsilon(1 + \epsilon)/2 \). The RG equations in Eq. (7) are very similar to that of the random transverse-field Ising chain, which is recovered with \( \kappa = 1 \). Both systems will scale to IRFP of that model for strong enough initial disorder and for \( \kappa > 0 \). Note, however, that for \( 0 < \kappa < 1 \), i.e. for \( q > 4 \) for the CM and \(-1 < \epsilon < 0 \) for the AT model, in some cases the generated new couplings/fields could be larger than the decimated ones, therefore the SDRG is not valid for weak disorder.

To see in detail the weak-to-strong disorder cross-over phenomena we perform a parallel numerical study about the critical behavior of the two models with varying degree of disorder. We use the DMRG method and calculate the average magnetization profiles, \( m_{z} \), fixing the spins at one boundary, \( s_{1} = 1 \), and \( \sigma_{l}^{z} = \tau_{l}^{z} = 1 \), respectively, whereas the spins at the other end of the chains, at \( l = L \), are free. In particular we consider the scaling of the magnetization for spins at the bulk, when \( l = L/2 \) and \( m_{b} \equiv m_{L/2} \), and that at the surface, when \( m_{s} \equiv m_{L} \):

\[ m_{b} \sim L^{-x}, \quad m_{s} \sim L^{-x^{'}} , \]

from which the scaling dimensions, \( x \) and \( x^{'} \) are calculated.

Useful information about the dynamical exponent, \( z \), can be obtained from the distribution function of the surface magnetization, which has the limiting behavior [2]:

\[ P(\ln m_{s}) \sim m_{s}^{1/z}, \quad m_{s} \to 0 . \]

The scaling exponent, \( z^{'} \), in Eq. (9) should be compared with that of due to pure quantum fluctuations, \( z_{q} = 1 \), and then \( z = \max(1, z^{'}). \)

For both models we perform the calculations at the self-duality point, which corresponds to the critical point of the pure systems, as well as, according to the SDRG analysis, to the fixed-points of the strongly disordered systems. By choosing the same distribution function, \( P(y)dy \), of the couplings \( J_{i} \) and that of the fields \( h_{i} \), we ensure to stay at the self-duality point and use the parametrization:

\[ P(y) = \Delta y^{-1+1/\Delta}, \quad 0 \leq y \leq 1, \quad 0 < \Delta < \infty . \]
One can see here that $\Delta$ plays the role of the strength of disorder: the pure system is recovered as $\Delta \to 0$, whereas as $\Delta \to \infty$ the distribution corresponds to that in the IRFP [1].

In the actual calculations we used $q = 5$ for the CM while for the AT model we took $\epsilon = -0.75$. The bulk and surface magnetizations are calculated on relatively large finite systems up to $L = 32$ and 10000 disorder realizations were used, except for the largest sizes of the AT model, when we have some 1000 samples. For stronger disorder, i.e. for larger $\Delta$ the energy gap in a typical sample is decreasing, therefore to maintain sufficient numerical accuracy of the code one needs to keep relatively more states in the DMRG procedure. As a consequence the computational demand of the calculation is strongly increasing with $\Delta$, therefore we have restricted ourselves to calculate only at few points in the strongly disordered regime. Generically the DMRG algorithm performs rather well for disordered systems, as it is known also from other several examples [24,12].

Next in Fig. 2 the scaling exponents of the average bulk and surface magnetization as a function of the strength of disorder for the two models we can extract a common route from the weak to strong disorder crossover, which is expected to be generally valid for a class of random critical quantum systems. This scenario is summarized in a generic RG phase diagram depicted in Fig. 3 in terms of the strengths of disorder, $\Delta$, and a model dependent parameter, say $\omega$, which is used to characterize points in a critical line, (c.f. $\omega = \epsilon$ for the AT model, $\omega = 4 - q$ for the CM and $\omega = q/2 - 1$ for the quantum Potts model). For $\omega \geq 0$ the system is in the strong disorder (SD) phase, where the IRFP is strongly attractive. In the other part of the phase diagram, for $\omega < 0$, there are two more phases: the weak disorder (WD) and the intermediate disorder (ID) regions. Here the SD part of the phase

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Plots of $1/z'$ vs. $\Delta$ for the random AT model with $\epsilon = -0.75$ (■) and for the CM with $q = 5$ (○). The limiting values of $\Delta_0$ and $\Delta_\infty$, where $1/z' = 1$ and $1/z' = 0$, respectively are model dependent. The error bars in the figure are due to finite size effects and disorder averaging.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Scaling exponents of the average bulk and surface magnetization as a function of the strength of disorder for the $q = 5$ CM (○) and for the AT model with $\epsilon = -0.75$ (■). The limiting values of the exponents, corresponding to that of the IRFP are denoted by dashed lines.}
\end{figure}

From the numerical and the SDRG results obtained for the two models we can extract a common route from the weak to strong disorder crossover, which is expected to be generally valid for a class of random critical quantum systems. This scenario is summarized in a generic RG phase diagram depicted in Fig. 3 in terms of the strengths of disorder, $\Delta$, and a model dependent parameter, say $\omega$, which is used to characterize points in a critical line, (c.f. $\omega = \epsilon$ for the AT model, $\omega = 4 - q$ for the CM and $\omega = q/2 - 1$ for the quantum Potts model). For $\omega \geq 0$ the system is in the strong disorder (SD) phase, where the IRFP is strongly attractive. In the other part of the phase diagram, for $\omega < 0$, there are two more phases: the weak disorder (WD) and the intermediate disorder (ID) regions. Here the SD part of the phase

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{Scaling exponents of the average bulk and surface magnetization as a function of the strength of disorder for the $q = 5$ CM (○) and for the AT model with $\epsilon = -0.75$ (■). The limiting values of the exponents, corresponding to that of the IRFP are denoted by dashed lines.}
\end{figure}
diagram is attracted by the IRFP, while the critical behavior in the WD regime is governed by the fixed points of the pure system, which are located at $\Delta = 0$. In the ID regime, where there is a competition between quantum fluctuations and disorder effects, dynamical scaling is anisotropic, $1 < z < \infty$, and the static and dynamical critical exponents are disorder dependent. At the boundaries of the ID region there are $1/z = 0$ and $1/z = 1$, respectively, while at $\Delta = 0$, i.e. in the pure system limit they are at $\omega = 0$ and $\omega = \omega_0$. In the latter case for the pure model with a parameter $\omega_0$ the Harris criterion in Eq. (3) is saturated, i.e. $\nu_0(\omega_0) = 2/d$.

![Image of phase diagram](image-url)

FIG. 3. Schematic RG phase diagram of a quantum spin system having a critical line parametrized by $\omega$, in the presence of disorder of strength, $\Delta$. For details see the text.

We believe that the above scenario is relevant for some higher dimensional systems and therefore could have experimental relevance, too. As an example we mention the two dimensional random transverse-field Ising model where by a numerical implementation of the SDRG method an IRFP is found [23], which is attractive for strong disorder both for spin-glasses (SG-s) and random ferromagnets (FM-s). In numerical studies, however, a finite dynamical exponent, $z$, is obtained for the SG model [24], while for the random FM $z$ is divergent at the critical point [2]. A possible explanation of this controversy is that the studied SG is still in the ID region, whereas the random FM is in the SD phase. Further examples could be provided by random antiferromagnetic spin systems: chains, ladders and 2d models, where often conventional fixed-point behavior is obtained [16,17,28].

The authors are grateful to R. Melin, H. Rieger and L. Turban for useful discussions. This work has been supported by a German-Hungarian exchange program (DAAD-MÖB), by the Hungarian National Research Fund under grant No OTKA T023642, T025139, T034183, F26004 and MO28418 and by the Ministry of Education under grant No FKFP 87/2001.

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