Griffiths-McCoy Singularities in Random Quantum Spin Chains: Exact Results through Renormalization

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(Received 22 May 2000)

The Ma-Dasgupta-Hu renormalization group (RG) scheme is used to study singular quantities in the Griffiths phase of random quantum spin chains. For the random transverse-field Ising spin chain we have extended Fisher's analytical solution to the off-critical region and calculated the dynamical exponent exactly. Concerning other random chains we argue by scaling considerations that the RG method generally becomes asymptotically exact for large times, both at the critical point and in the whole Griffiths phase. This statement is checked via numerical calculations on the random Heisenberg and quantum Potts models by the density matrix renormalization group method.

DOI: 10.1103/PhysRevLett.86.1343 PACS numbers: 75.50.Lk, 05.50.+q, 64.60.Ak, 68.35.Rh

In a random quantum system at zero temperature several physical quantities are singular not only at the critical point, but in a whole region as well, which extends on both sides of the transition point [1]. In this Griffiths phase [2] a random quantum system is noncritical in the space direction (spatial correlations decay exponentially), whereas it is critical in the time direction and the corresponding behavior due to Griffiths-McCoy singularities [2,3] is controlled by a line of semicritical fixed points characterized by the dynamical exponent $z(\delta)$, which depends on the value of the quantum control parameter δ. For example, average autocorrelations decay in (imaginary) time τ as $\sim\tau^{-z(\delta)}$; for a small magnetic field $H \to 0$, the magnetization behaves as $\sim H^{1/z(\delta)}$; the low temperature susceptibility and specific heat are singular as $\sim T^{1/z(\delta)-1}$ and $\sim T^{1/z(\delta)}$, respectively.

In an experimental point of view the $LiHo_xY_{1-x}F_4$ system, where magnetic Ho^{3+} atoms are randomly substituted by nonmagnetic Y^{3+} atoms, in the presence of a longitudinal magnetic field H_z is a quantum spin glass [4]. The effective Hamiltonian of the system is a random transverse-field Ising model (RTIM), where the quantum control-parameter is H_z^2. Heisenberg spin chains with random ferromagnetic couplings are realized by the NMP-TCNQ (N-methyl-phenazinium tetracyanoquinodimethanide) [5]. Griffiths-McCoy singularities are also used to provide a theoretical explanation about the non-Fermi liquid behavior in U and Ce intermetallics [6]. In these systems an effective Hamiltonian in the form of the RTIM can be obtained from the random Kondo model in the limit of strong anisotropy.

Among the theoretical methods developed to study random quantum systems the renormalization group (RG) scheme introduced by Ma, Dasgupta, and Hu [7] plays a special role. For a class of systems, the critical behavior of those is controlled by an infinite-randomness fixed point [8] (IRFP), the RG method becomes asymptotically exact during iteration. For some one-dimensional models, such as the RTIM [9] and the random XXZ model [10], Fisher has obtained analytical solution of the RG equations and in this way many new exact results and new physical insights about the critical behavior of these models have been gained. Subsequent analytical [11] and numerical [11,12] investigations of the models are in agreement with Fisher's results. The RG scheme has been numerically implemented in higher dimensions [8,13], as well, to study the critical behavior of the RTIM, and reasonable agreement with the results of quantum Monte Carlo simulations [14] has been found. Considering the Griffiths phase of random quantum spin chains here the RG scheme has been rarely used [13], mainly due to the general belief that the method looses its asymptotically exact properties by leaving the vicinity of the scale invariant critical point.

Our aim in the present Letter is to clarify the applicability of the Ma-Dasgupta-Hu RG method in the Griffiths phase of random quantum spin chains. We start with the RTIM, extend Fisher's calculation [9] to the Griffiths phase of the model, and present the analytical solution of the RG equations. Then, for general models, we analyze by scaling considerations the structure of the RG equations around the line of semicritical fixed points and arrive at the conclusion that the RG method becomes asymptotically exact in the whole Griffiths region. This statement is then checked numerically on the random Heisenberg chain and the random quantum Potts model (RQPM) using the density matrix renormalization group (DMRG) method.

We start with the 1D RTIM which is defined by the Hamiltonian

$$\mathrm{H}_I = -\sum_i J_i \sigma_i^x \sigma_{i+1}^x - \sum_i h_i \sigma_i^z, \qquad (1)$$

where the $\sigma_i^{x,z}$ are Pauli matrices at site i and J_i and h_i are the couplings and the transverse fields, respectively, which are independent random variables. The quantum control-parameter of the model is defined as

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

where var$[x]$ is the variance of x and we use $[\cdots]_{\rm av}$ to denote averaging over quenched disorder. For $\delta > 0$ ($\delta < 0$) the system is in the paramagnetic (ferromagnetic) phase, so that the random quantum critical point is at $\delta = 0$.

In the Ma-Dasgupta-Hu RG method the strongest term in the Hamiltonian, coupling, or field, of strength Ω is successively decimated out and the neighboring fields or couplings are replaced by weaker ones, which are generated by a perturbation calculation. The basic RG equations for coupling and field decimations are given by

$$\tilde{h} = \frac{h_i h_{i+1}}{J_i \kappa}, \qquad \tilde{J} = \frac{J_{i-1} J_i}{h_i \kappa}, \tag{3}$$

respectively, which are related through duality. Here, for the RTIM $\kappa = 1$. Under renormalization we follow the probability distributions of the couplings $R(J, \Omega)$, and that of the fields $P(h, \Omega)$. When the energy scale is lowered as $\Omega \to \Omega - d\Omega$ the distribution of the couplings is changed as

$$\begin{aligned}\frac{dR(J,\Omega)}{d\Omega} &= R(J,\Omega)[P(\Omega,\Omega) - R(\Omega,\Omega)] \\ &\quad - P(\Omega,\Omega)\int_{J\kappa}^{\Omega} dJ' R(J',\Omega) \\ &\quad \times R\left(\frac{J\Omega\kappa}{J'},\Omega\right)\frac{\Omega\kappa}{J'},\end{aligned} \tag{4}$$

where the first term on the right-hand side is due to a balance between decimated couplings and normalization, whereas the second term accounts for the generated new couplings. A similar equation for the field distribution follows from Eq. (4) through duality, which amounts to interchange $J \leftrightarrow h$ and $R \leftrightarrow P$.

For the RTIM, i.e., for $\kappa = 1$, we found one class of solutions of the RG equations in the form

$$\begin{aligned}R(J,\Omega) &= R(\Omega,\Omega)(\Omega/J)^{1-R(\Omega,\Omega)\Omega}, \\ P(h,\Omega) &= P(\Omega,\Omega)(\Omega/h)^{1-P(\Omega,\Omega)\Omega},\end{aligned} \tag{5}$$

where the distributions involve the parameters $\tilde{R}(\Omega) \equiv R(\Omega,\Omega)$ and $\tilde{P}(\Omega) \equiv P(\Omega,\Omega)$, which satisfy the ordinary differential equations $d\tilde{R}/d\Omega = -\tilde{R}/\Omega + \tilde{P}\tilde{R}$ and $d\tilde{P}/d\Omega = -\tilde{P}/\Omega + \tilde{P}\tilde{R}$, consequently $(\tilde{P} - \tilde{R})\Omega = 1/z = {\rm const}$. Thus the solution is characterized by one parameter, $z = z(\delta)$, which depends on the quantum control-parameter δ: at the critical point, $1/z(0) = 0$, whereas in the paramagnetic phase, $\delta > 0$, $1/z(\delta) > 0$ and monotonically increases with δ.

In terms of the variables, $y = \tilde{R}\Omega + 1/2z = \tilde{P}\Omega - 1/2z$ and $x = -\ln\Omega$ we arrive at the differential equation

$$\frac{dy}{dx} + y^2 = \frac{1}{4z^2}, \tag{6}$$

which has the solution $y = 1/(x - x_0)$, $x_0 = {\rm const}$, *at the critical point* with $1/z = 0$. The distribution of $\rho = R\Omega$ in terms of the variable $\eta = -(\ln\Omega - \ln J)/\ln\Omega$ is given by $\rho(\eta)d\eta = \exp(-\eta)d\eta$, which corresponds to the fixed-point solution by Fisher [9]. At this point we refer to Fisher's analysis [9] and conclude that the functions in Eqs. (5) indeed represent the fixed-point distribution for all nonsingular initial distributions.

In the Griffiths phase $\delta > 0$, the solution of Eq. (6) in terms of the original energy-scale variable Ω is given by

$$y = \frac{y_0/2z + 1/4z^2 \tanh[\ln(\Omega_0/\Omega)/2z]}{1/2z + y_0 \tanh[\ln(\Omega_0/\Omega)/2z]}, \tag{7}$$

where $y = y_0$ at a reference point $\Omega = \Omega_0$. Approaching the line of semicritical fixed points, i.e., for $\Omega/\Omega_0 \to 0$, we have to leading order:

$$\begin{aligned}\tilde{R}\Omega &= \tilde{P}\Omega - 1/z \\ &= \tilde{R}(\Omega_0)/[\tilde{P}(\Omega_0)z](\Omega/\Omega_0)^{1/z} + \cdots,\end{aligned} \tag{8}$$

thus $\tilde{P}$ and $\tilde{R}$ have different low energy asymptotics.

The *physical relevance* of $1/z$ can be obtained by studying the change of number of spins, $n_\Omega \to n_\Omega - dn_\Omega$ connected with a change in the energy scale as $\Omega \to \Omega - d\Omega$. This leads to the differential equation $dn_\Omega/d\Omega = n_\Omega[P(\Omega,\Omega) + R(\Omega,\Omega)]$, the solution of which is given by

$$\begin{aligned}n_\Omega &= \{\cosh[\ln(\Omega_0/\Omega)/2z] \\ &\quad + 2zy_0 \sinh[\ln(\Omega_0/\Omega)/2z]\}^{-2},\end{aligned} \tag{9}$$

which along the line of semicritical fixed points has the asymptotic behavior $n_\Omega = {\rm const}\Omega^{1/z}$, $\Omega \to 0$. Since the typical distance between remaining spins is $L_\Omega \sim 1/n_\Omega \sim \Omega^{-1/z}$, we can identify z as the *dynamical exponent,* which governs the relation between time scales and length scales as $\tau \sim L^z$.

Next we show that z is invariant along the RG trajectory and can be deduced from the original distributions. For this we consider the averages $[J^\mu]_{\rm av}$ and $[h^{-\mu}]_{\rm av}$, and using Eq. (4) and its dual we calculate the derivative

$$\begin{aligned}\frac{d}{d\Omega}[(J/h)^\mu]_{\rm av} &= (1 - [(J/h)^\mu]_{\rm av}) \\ &\quad \times [P(\Omega,\Omega)\Omega^{-\mu}[J^\mu]_{\rm av} \\ &\quad + R(\Omega,\Omega)\Omega^\mu[h^{-\mu}]_{\rm av}],\end{aligned} \tag{10}$$

which is vanishing for $\mu = \tilde{\mu}$, if $[(J/h)^{\tilde{\mu}}]_{\rm av} = 1$. Consequently, $\tilde{\mu}$ stays invariant along the RG trajectory until the fixed point, where using the distribution in Eqs. (5) we obtain $\tilde{\mu} = 1/z$. Thus the dynamical exponent for the RTIM is given by the solution of the equation:

$$[(J/h)^{1/z}]_{\rm av} = 1, \tag{11}$$

which is then exact, since the RG transformation becomes asymptotically exact as $\Omega \to 0$. This latter statement follows from the fact that the ratio of decimated bonds, Δn_J,

and decimated fields, Δn_h, goes to zero as $\Delta n_J/\Delta n_h = R(\Omega,\Omega)/P(\Omega,\Omega) \sim \Omega^{1/z}$. Then the probability $\Pr(\alpha)$ that the value of a coupling J being neighbor to a decimated field is $\Omega > J > \alpha\Omega$ with $0 < \alpha < 1$ is given by $\Pr(\alpha) = 1 - \alpha^{\tilde{R}\Omega}$, which goes to zero for any nonzero α, since $\tilde{R}\Omega \sim \Omega^{1/z}$ at the fixed point. Consequently, the decimations in Eq. (3) and the related RG equation in Eq. (4) and its dual are indeed exact.

The relation in Eq. (11) can be recovered starting from the exact expression for the surface magnetization m_s on a chain with a fixed spin at site $L + 1$ [11,15]:

$$\frac{1}{m_s^2} = 1 + \sum_{l=1}^{L} \prod_{i=1}^{l} \left(\frac{h_i}{J_i}\right)^2. \tag{12}$$

This type of expression is the so-called Kesten variable in the mathematical literature [16] and the corresponding probability distribution is singular at $m_s = 0$ in the thermodynamic limit for $[\ln J]_{\rm av} > [\ln h]_{\rm av}$ [16,17]. Then for the distribution of $\ln m_s$ we have the following singularity:

$$P(\ln m_s) \sim m_s^{1/\tilde{z}}, \qquad m_s \to 0\,, \tag{13}$$

where $\tilde{z}$ is the solution of Eq. (11) in terms of the dual variables. The physical origin of the small m_s tail of the distribution is due to such samples which have a weakly coupled domain (WCD), which effectively cuts the system into two very weakly interacting parts and thus reduces the surface order enormously. In the dual system in the paramagnetic phase the dual object to a WCD is a strongly coupled domain (SCD) which results in a very small energy gap ϵ. Thus in the tails of the distributions, m_s and ϵ are dual quantities. This remark indicates that the dynamical exponent found by the RG calculation in Eq. (11) is indeed exact [18].

We note that the Hamiltonian in Eq. (1) is equivalent to the transfer matrix of a randomly layered 2D classical Ising model, the McCoy-Wu (MW) model [19], in the strong anisotropy limit and the random couplings (transverse fields) are related to the original random horizontal (vertical) bonds. In the MW model there is a Griffiths phase where correlations in the vertical direction have a power law form with a decay exponent which is related to $z(\delta)$ in Eq. (11).

Next, we consider general random quantum spin chains with a critical IRFP and analyze the structure of the RG equations close to the line of semicritical fixed points, thus as $\Omega \to 0$. As for the RTIM, the decimation for fields and couplings is asymmetric and for $\Omega \to 0$ exclusively fields are decimated out, which are typically infinitely stronger, than the neighboring couplings. Therefore the RG decimation equations in Eq. (3) are asymptotically exact. The second point is to show that the dynamical exponent stays invariant along the RG trajectory, even though in the starting phase the RG equations are approximative. For this we consider the low energy tail of the distribution function of the first gap $P_1(\ln\epsilon)$, which involves in analogy to Eq. (13) the exponent z, and uses the scaling result of Ref. [20]. This states that the probability distribution of the second, third, etc. gaps are related to $P_1(\ln\epsilon)$ as $P_2(\ln\epsilon) \sim P_1^2(\ln\epsilon)$, $P_3(\ln\epsilon) \sim P_1^3(\ln\epsilon)$, etc., due to the fact that for a small second, third gap one needs two, three independent SCDs and the corresponding probabilities are multiplied. In the RG decimation, the SCDs are eliminated only through coupling decimation, since their couplings are stronger than the average fields. If at some time a SCD with a small gap ϵ is eliminated, then in the probability distribution $P_1(\ln\epsilon)$ one should consider the former second gap and use the corresponding conditional probability, $P_1(\ln\epsilon) \to P_2(\ln\epsilon)/P_1(\ln\epsilon) \sim P_1(\ln\epsilon)$. Thus the small energy tail of the gap distribution and, consequently, the dynamical exponent, remains invariant under the renormalization procedure. The previously obtained exact results for the RTIM give strong support for the validity of these phenomenological considerations.

For a numerical demonstration of the validity of the above statement we considered two random quantum spin chains, the dimerized Heisenberg (XXX) chain and the q-state RQPM, both having a set of RG equations very similar to that of the RTIM in Eq. (3). For the dimerized XXX chain, J and h in Eq. (3) are replaced by the Heisenberg couplings at odd and even positions, J_o and J_e, respectively, and the parameter takes the value $\kappa = 2$ [7,10]. The distance from the critical point is measured similarly to Eq. (2). For the q-state, RQPM fields and couplings play an analogous role as for the RTIM, the quantum control-parameter is given in Eq. (2), whereas κ takes the value $\kappa = q/2$ [21]. We note that the RG equations for the XXX chain and the $q = 4$ state RQPM are identical.

At the critical point, the RG equations for $1 \le \kappa < \infty$ have been solved by Senthil and Majumdar [21] with the result that κ is an irrelevant variable and the IRFP is the same as for the RTIM. In the Griffiths phase we could not find a complete solution of the RG equations, in spite of the close similarity to that of the RTIM. We could, however, show that up to an accuracy of $O(\Omega^{1/z})$ the solution is of the form of Eqs. (5) and thus there is infinite randomness along the line of fixed points. The z exponent, however, does depend on the parameter κ, since the validity of the condition in Eq. (11) is limited to $\kappa = 1$, thus in general $z = z_\kappa(\delta)$.

We have calculated the dynamical exponent by a numerical implementation of the RG scheme over 50 000 samples of length $L \le 2^{14}$. Starting with the uniform probability distribution: $R_0(J) = \Theta(1 - J)\Theta(J)$, $P_0(h) = \Theta(h_0 - h)\Theta(h)/h_0$ (and analogously for the XXX chain) we got the estimates shown in Fig. 1: $1/z_\kappa$ is a monotonously decreasing function of κ and eventually it goes to zero in the whole Griffiths phase in the limit $\kappa \to \infty$, which follows from an analysis of Eq. (4).

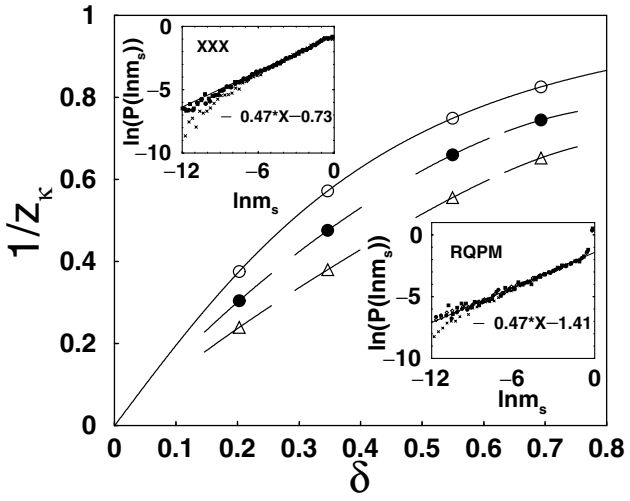

FIG. 1. Dynamical exponents from numerical iteration of the RG equations in Eq. (3). For $\kappa = 1$ (○), which corresponds to the RTIM and the random dimerized XX chain, the exact result is given by the full line, for $\kappa = 2$ (●) and 4 (△) the broken lines are a guide to the eye. Insets: Probability distribution of the logarithm of the surface magnetization of the dimerized random XXX chain and the $q = 4$ state RQPM both with $\delta = -(\ln 2)/2$ for different finite systems [$L = 8$ (×), $L = 16$ (●), $L = 32$ (■), $L = 64$ (◇)] calculated by the DMRG method. The full straight lines with the same slope, $1/z(\delta) = 0.47$, represent the asymptotic behavior according to the RG method, as given in the main figure. The accuracy of the estimate of $1/z(\delta)$ is about a few percent in both cases and $1/z(\delta)$ is considerably smaller than the linear estimate by Fisher [9]: $1/z(\delta) \approx 2|\delta| = \ln 2$.

The dynamical exponents of the XXX chain and the RQPM are also calculated directly from the asymptotic behavior of the distribution of the surface magnetization, as given in Eq. (13). For the numerical calculations of the surface magnetizations we used the DMRG method for rather large finite chains with $L \leq 64$ and considered some 20 000 samples. We found an overall agreement between the dynamical exponents calculated by the two methods. As a demonstration we show in the insets of Fig. 1 the distribution of m_s for the XXX chain, compared with that of the $q = 4$ state RQPM, where for both models we are at the same distance from the transition point. As seen in Fig. 1 the asymptotic behavior of the two distributions is identical, as expected on the RG basis, since $\kappa = 2$ for both models. Furthermore the dynamical exponents agree very well with those calculated by the RG method.

To conclude, we have shown in this paper that for random quantum spin chains the RG method of Ma, Dasgupta, and Hu is asymptotically exact for large times, i.e., along the line of semicritical fixed points. This type of exactness of the procedure follows from the fact that the fixed-point distribution of the couplings is infinitely broad and that the dynamical exponent is invariant during the iteration process. A possible way to control the error during iteration, i.e., as Ω is decreased towards zero, is to consider larger and larger blocks in the decimation and follow the change of the distribution functions numerically. Our result will hopefully stimulate new efforts to solve the RG equations for different systems analytically in 1D also outside the critical point, and in higher dimensions to perform numerical calculations and get more precise estimates for the Griffiths-McCoy singularities.

This work has been supported by the Hungarian National Research Fund under Grant No. OTKA TO23642, TO25139, F/7/026004, MO28418, and by the Ministry of Education under Grant No. FKFP 0596/1999. We are indebted to E. Carlon for his participation in the early stages of the DMRG calculations. F. I. is grateful to H. Rieger and L. Turban for previous cooperation in the project and for useful discussions.

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