Activated scaling in disorder rounded first-order quantum phase transitions

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First-order phase transitions, classical or quantum, subject to randomness coupled to energy-like variables (bond randomness) can be rounded, resulting in continuous transitions (emergent criticality). We study perhaps the simplest such model, quantum three-color Ashkin-Teller model and show that the quantum critical point in $(1+1)$ dimension is an unusual one, with activated scaling at the critical point and Griffiths-McCoy phase away from it. The behavior is similar to the transverse random field Ising model, even though the pure system has a first-order transition in this case. We believe that this fact must be attended to when discussing quantum critical points in numerous physical systems, which may be first-order transitions in disguise.

The effect of quenched randomness on thermodynamic properties could be varied. The systems that behave less and less random at larger and larger length scales, i.e., the randomness averages out, are described by pure fixed points. On the other hand, if the randomness is competitive at all scales, the system is controlled by random fixed point and the properties of the system is altered by rare spatially localized active regions [1]. In the extreme limit, the fixed point is captured by the infinite randomness fixed point: the main features are a strong dynamical anisotropy and a broad distribution of physical quantities which is manifest through drastically different average and typical correlation functions. Some example of such systems are the quantum critical point of random quantum Ising and Potts models [2,5], the random singlet states of certain random antiferromagnetic spin chains [6,7], quantum critical points separating random singlet states and the Ising antiferromagnetic phase, or the Haldane state in the random spin-1 Heisenberg chain [3].

In addition to the singularities of the thermodynamic quantities at the quantum critical point, there is a whole parameter range around the phase transition point in which physical observables display singular and even divergent behavior in spite of a finite correlation length [4]. Within this Griffiths-McCoy phase, there is a continuously varying dynamical exponent, $z$, that relates the scale of energy and length via $\xi \propto \tau^{1/z}$, with $z$ diverging as $z \propto \delta^{-\psi\nu}$. Here, $\delta$ is the deviation from the critical point, $\psi$ is some dimensionless positive constant, and $\nu$ is the correlation length exponent. A signature of the existence of infinite randomness fixed point is the divergence of the dynamical critical exponent $z$ at the critical point, $\delta = 0$. In that case, the system exhibits activated dynamical scaling, $\xi_\tau \propto e^{c_{\text{const}} \times \xi^{1/z}}$, where $\xi_\tau$ represents a characteristic time scale of the system.

Both quantum and classical first-order phase transitions are ubiquitous in nature, because they do not require fine tuning of a control parameter of the system. Understanding the effect of quenched randomness that couples to energy-like variables on the thermodynamic properties of the systems that exhibit a first-order phase transition has been a challenge of experimental and theoretical studies for many years [13].

Here we investigate the effect of quenched disorder on the quantum three-color Ashkin-Teller model in $(1+1)$ dimension, which exhibits a first-order quantum phase transition in the absence of impurities. We employ discrete-time quantum Monte-Carlo method. Because there is no frustration in this system, we are able to use highly efficient cluster algorithms [17]. Surprisingly to us, for this disorder rounded quantum critical point, we find activated scaling at criticality and the off-critical region is characterized by Griffiths-McCoy singularities.

The Hamiltonian of the $N$-color quantum Ashkin-Teller model in $(1+1)$ dimension is given by [13]

$$H = -\sum_{\alpha=1}^{N} \sum_{i=1}^{L} (J_{2,i}(\sigma_{\alpha,i}^{\beta} \sigma_{\alpha,i+1}^{\gamma} + h_{1,i}\sigma_{\alpha,i}^{\alpha}))$$

$$-\sum_{\alpha<\beta=1}^{N} \sum_{i=1}^{L} (J_{4,i}(\sigma_{\alpha,i}^{\alpha} \sigma_{\alpha,i+1}^{\beta} \sigma_{\beta,i}^{\beta} + h_{2,i}\sigma_{\alpha,i}^{\beta} \sigma_{\beta,i}^{\beta})),$$

where $L$ is the length of the lattice, Greek sub-indices denote the colors, Latin sub-indices denote the lattice sites, and $\sigma^\alpha$’s are the Pauli operators. The $J_{2,i}$ and $J_{4,i}$ are the random nearest-neighbor coupling constants. The $h_{1,i}$ and $h_{2,i}$ are the random transverse fields. The random coupling constants and the transverse fields are taken from a distribution restricted to only positive values. The model is self-dual, which amounts to the invariance of the Hamiltonian in Eq. (1) under the transformation $J_{2,i} \leftrightarrow h_{1,i}$, $J_{4,i} \leftrightarrow h_{2,i}$, $\mu_{\alpha,i} \leftrightarrow \sigma_{\alpha,i}^{\alpha} \sigma_{\alpha,i+1}^{\alpha}$, and $\sigma_{\alpha,i}^{\alpha} \leftrightarrow \mu_{\alpha,i} \mu_{\alpha,i+1}^{\alpha}$, where $\mu$’s are the dual Pauli operators. The pure version of this model has been studied in the past. It is known that for $N \geq 3$, $J_{4,i}/J_{2,i} \geq 0$ and $h_{2,i}/h_{1,i} > 0$, there is a first-order phase transition from a paramagnetic to an ordered state [23].

To study the $d$-dimensional quantum Hamiltonian in Eq. (1), we propose an effective classical model in $(1+1)$ dimension, where the extra imaginary time dimension is of size $\beta \equiv 1/T$ and is divided up into $L_\tau \equiv \beta/\Delta \tau$ intervals each of width $\Delta \tau$ in the limit $\Delta \tau \rightarrow 0$. We introduce disorder only in the horizontal direction. This emulates a quenched disordered quantum system whose disorder is perfectly correlated in the imaginary time direction. Hence, we expect the behavior of this system to be in the universality class as the original quantum Ashkin-Teller model in Eq. (1). This procedure is the same as the McCoy-Wu random Ising model [2,9], which is shown to be equivalent to the random transverse field quantum spin-$1/2$ Ising model in the large imaginary time limit.
The partition function is $Z = \lim_{\Delta \tau \to 0} \text{Tr} e^{-S}$, with the proposed effective action given by

$$S = - \sum_{\alpha, \tau, i} J_i S_{\alpha, i}(\tau) S_{\alpha, i+1}(\tau) - \sum_{\alpha, \tau, i} J S_{\alpha, i}(\tau) S_{\alpha, i}(\tau + 1) - \sum_{\alpha \neq \beta, \tau, i} K_i S_{\alpha, i}(\tau) S_{\beta, i}(\tau) S_{\alpha, i+1}(\tau) S_{\beta, i+1}(\tau) - \sum_{\alpha \neq \beta, \tau, i} K S_{\alpha, i}(\tau) S_{\alpha, i}(\tau + 1) S_{\beta, i}(\tau) S_{\beta, i}(\tau + 1), \quad (2)$$

where the $S_i(\tau) = \pm 1$ are classical Ising spins, the indices $\alpha$ and $\beta$ denote the colors, the index $i$ runs over the sites of the one-dimensional lattice, and $\tau = 1, 2, \ldots, L_\tau$ denotes a time slice. For computational convenience, we set $\Delta \tau = 1$ and equivalently take the limit $L_\tau \to \infty$ implying $T \to 0$. The two- and four-spin couplings, $J$ and $K_i$, are independent of $\tau$, because they are quenched random variables. We independently take the couplings $J_i$ and $K_i$ from the following rectangular distributions

$$\pi(J_i) = \begin{cases} 1, & \text{if } J - \frac{|J|}{2} < J_i < J + \frac{|J|}{2} \\ 0, & \text{otherwise} \end{cases} \quad \rho(K_i) = \begin{cases} 1, & \text{if } K - \frac{|K|}{2} < K_i < K + \frac{|K|}{2} \\ 0, & \text{otherwise} \end{cases} \quad (3)$$

In our Monte-Carlo simulation on a square lattice of size $L \times L_\tau$ we use periodic boundary conditions in both spatial and imaginary time directions. The equilibration “time” is estimated using the logarithmic binning method, i.e., we compare the average values of each observable over $2^n$ Monte-Carlo steps and make sure that the last three averages are independent indicating that the system is at the critical point.

For $J_{1,i}/J_{2,i} = h_{2,i}/h_{1,i} = 0$, the Hamiltonian (1) reduces to $N$ copies of the random transverse field quantum spin-$1/2$ Ising model. Our action in Eq. (2), in this limit, also reduces to $N$ copies of the well known classical McCoy-Wu model [7] whose critical point is given by

$$2J + \int_0^\infty dJ' P(J') \ln(\tanh(J')) = 0. \quad (4)$$

We first studied the McCoy-Wu model in some detail to confirm our Monte Carlo method.

First, we estimate the location of the quantum critical point along the analysis of Rieger and Young [29] for the quantum spin glass systems using the magnetic Binder cumulant [30]

$$V_m = 1 - \frac{(m^4)}{3(m^2)^2}, \quad (5)$$

where

$$m = \frac{1}{L_\tau L} \left[ \left\langle \sum_{\alpha} |m_{\alpha}| \right\rangle \right], \quad (6)$$

with $m_{\alpha} = \sum_{\tau} S_{\alpha, i}(\tau)$. The square and angular brackets, $[\cdots]$ and $\langle \cdots \rangle$, denote the disorder and thermal averages, respectively. In the disordered phase, $V_m \propto L^{-d} \to 0$ as $L \to \infty$ [31]. In the ordered phase, we have spontaneous magnetization at $\pm m$ and $V_m \to 2/3$ as $L \to \infty$ [31]. Furthermore, in the paramagnetic phase, for small $\tau$, the system is disordered and effectively classical at a finite temperature, therefore $V_m \to 0$. For $\tau \to \infty$, the system is quasi one-dimensional in the imaginary time direction, therefore $V_m \to 0$ also. There exists an intermediate point where $V_m$ acquires a maximum value $V_m^{\text{max}}$. This maximum value decreases as $L$ increases if the system is in the paramagnetic phase, whereas it increases as $L$ increases if the system is in the ferromagnetic phase. Therefore, there is an intermediate point at which the $V_m^{\text{max}}$ is a constant for all $L$ which is the quantum critical point (Fig. 1). For our model with the parameter set $(K, \Delta K, \Delta J) = (0.08, 0.04, 0.2)$, we estimate the critical point to be $J_c = 0.247 \pm 0.001$.

We obtain a second estimate of the critical point as follows: for any finite $L_\tau \propto 1/T$, the system is classical and the Binder cumulant has the finite size scaling of the form [30]

$$V_m = V (J - J_c) \frac{L^{1/\nu}}{L_\tau^{1/z}}. \quad (7)$$

Hence, for $J = J_c$ all curves cross at a single point. We find the critical point for a few finite temperature values and extrapolate $L_\tau \to \infty$ to obtain the location of the zero temperature quantum critical point as shown in Fig. 2. We obtain $J_c = 0.242 \pm 0.001$, close to the previous value.
We also found the critical point of the system with the parameter set \((K, \Delta K, \Delta J) = (0.1, 0.05, 0.2)\), with \(J_c = 0.205 \pm 0.002\) from the first method and \(J_c = 0.202 \pm 0.005\) from the second method. Careful analyses of two parameter sets \((K, \Delta K, \Delta J) = (0.08, 0.04, 0.2)\) and \((0.1, 0.05, 0.2)\) yielded very similar results. Henceforth, we will be reporting only on the former parameter set in the rest of our paper. In a future publication, we expect to present results for other parameter sets as well.

According to the finite-size scaling in Eq. (7), at the critical point, \(V_m\) is independent of \(z\). Therefore, a plot of the \(V_m\) against \(L \tau / L_{\max}^{\psi}\) at the critical point should collapse the data, but from Fig. 3 we see that it does not. In contrast, if we assume that the logarithm of the characteristic time scale is a power of the length scale, as in the quantum spin-

The equal time correlation function \(C_{\alpha,i}(r) = \left\langle [S_{\alpha,i}(\tau) S_{\alpha,i+r}(\tau)] \right\rangle\) is calculated at criticality for spins \(r = L/2\) apart. As shown in Fig. 4, the distribution of the correlation function, \(P(C(L/2))\), is getting broader and broader as \(L\) increases. This indicates that the rare events dominate the critical properties of the system. As a result of the breadth of the distribution, the average and typical quantities behave differently. The typical correlation function is defined here as the exponential of the average of the logarithm \(\ln \chi_{\alpha,i}^{\max}\). In Fig. 5, we show that the average correlation function, \(C_{\text{avg}}(L/2)\), falls off as a power law, \(C_{\text{avg}}(r) \propto r^{-\eta}\), whereas the typical correlation, \(C_{\text{typ}}(L/2)\), has a downward curvature and falls off faster than the average value. Our result is consistent with the existence of a stretched exponential decay, \(C_{\text{typ}}(r) \propto e^{-c r^{\eta}}\), at the critical point.

We now turn our attention to off-critical region and calculate the linear susceptibility, \(\chi_l\), in the disordered phase, \(J < J_c\). In the imaginary time formalism \(\chi_l = \sum_{\tau=1}^{L_{\tau}} \langle S_{\alpha,i}(0) S_{\alpha,i}(\tau) \rangle\). The dynamical exponent, \(z\), can be calculated from the probability distribution distribution of linear local susceptibility. Away from the critical point the distributions for different system sizes are well localized and they get narrower as \(L\) increases, while close to the critical point the probability distribution of \(\ln \chi_{\alpha,i}^{\max}\) gets broader with \(L\); see Fig. 6. This broadening of the probability distribution is a strong support for the existence of strongly coupled rare regions in the vicinity of the critical point.
FIG. 4. (Color online) A plot of the distribution of the equal-time correlation of spins $L/2$ apart for the parameter set $(K, \Delta_K, \Delta_J) = (0.08, 0.04, 0.2)$ at $J_c = 0.242$. One sees that the distribution gets broader and broader as $L$ increases. For this plot we used $10^5$ realizations of disorder.

If $P(\ln \chi_l)$ has a power law tail with $P(\ln \chi_l) \propto \chi_l^{-d/z}$, then its integral, $Q(\ln \chi_l)$ behaves similarly to $P(\ln \chi_l)$ with $\frac{d}{z} = 1$

\[
\ln[Q(\ln \chi_l)] = -\frac{d}{z} \ln \chi_l + \text{const.} \tag{8}
\]

It is more accurate to extract the exponent, $z$, from the cumulative distribution, $Q(\ln \chi_l)$. In Fig. 5 we show the cumulative distribution of the logarithm of local linear susceptibility.

The average local susceptibility

\[
\chi_l^{(\text{avg})} = \int d\chi_l \chi_l P(\chi_l) = \int d\chi_l \chi_l^{-d/z} \tag{9}
\]

diverges, however, when $\frac{d}{z} \leq 1$. In Fig. 7 we show $\frac{d}{z}$ as a function of $J$ in the paramagnetic phase. We see that the value of $\frac{d}{z}$ is larger than 1 for a wide range of $J$ which indicates the divergence of the average local susceptibility in this region; also $\frac{d}{z} \to \infty$ as $J \to J_c \approx 0.242$, compatible with activated dynamical scaling at the criticality.

For a continuous phase transition, the Griffiths-McCoy phase is bounded above and below by the clean and disordered critical points, $J_c^0 < J < J_c$. In the present case, the pure system is not critical. We suggest, however, that the Griffiths-McCoy phase to be the region for which $\chi_l^{(\text{avg})}$ is not anticipated in the past and stands out as an example where the effect of disorder in a system is quite complex and considerable care must be exercised in analyzing quantum critical points where material disorder is inevitable.

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FIG. 7. (Color online) The dynamical exponent $z$, for different values of $J$ in the paramagnetic phase for the parameter set $(K, \Delta K, \Delta_j) = (0.08, 0.04, 0.2)$ for our largest lattice size $L = 32$. The blue vertical dashed line is the location of the induced quantum critical point. The horizontal dashed line corresponds to $z = 1$.

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