Quantum Phase Transitions in Random Magnets

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This talk will discuss novel critical behavior and "Griffiths-McCoy" singularities (which occur away from criticality) near quantum phase transitions in disordered systems with discrete (Ising) symmetry. One finds that distributions of many quantities are very broad, so it is insufficient to simply take the average. After reviewing some exact results in one-dimension obtained using a real space renormalization group approach, I will discuss extensions of these results obtained by a numerical method in which the spin problem is mapped on to free fermions. In this way, whole distributions can be determined with precision. The talk will then describe quantum Monte Carlo simulations which show that similar results also occur in higher dimensions, at least for $d = 2$.

Quantum phase transitions occur at $T = 0$, driven by quantum, rather than thermal, fluctuations as some parameter in the system is varied. Until recently, such transitions have received less attention than the more conventional "thermal" phase transitions where one goes through the transition by varying the temperature. However, there has recently been an upsurge of interest in quantum phase transitions, partly because there are experiments, and partly because, *in the presence of quenched disorder*, such transitions exhibit new physics which is rather poorly understood. An excellent general reference for Quantum Phase Transitions is the recent book by Sachdev [1].

Let us first discuss why one can generally set $\hbar = 0$ in treatments of critical phenomena. The thermal energy per degree of freedom is $k_B T$, where k_B is Boltzmann's constant, while the zero-point quantum of energy is $\hbar\omega_c$, for a fluctuation of characteristic frequency ω_c. As one approaches a phase transition, the correlation length, ξ, generally diverges with a power law, *i.e.*

$$\xi \sim \delta^{\nu} , \tag{1}$$

where δ is the deviation from criticality. As the critical point is approached, not only do the fluctuations extend over large spatial scales, they also become very slow, and there is a divergent relaxation time τ. This effect is known as critical slowing down. It is conventional [2] to define a dynamical exponent, z, by

$$\tau \sim \xi^{z} \ . \tag{2}$$

The appropriate quantum of energy is then $\hbar\omega_c$ with $\omega_c \sim 1/\tau$. Hence, if the transition is at a finite temperature, T_c, quantum mechanics is irrelevant for critical phenomena, *i.e.* $\hbar\omega_c \ll k_B T$, provided

$$\delta \ll T_c^{1/z} \ , \tag{3}$$

which is *always* satisfied sufficiently close to T_c, *provided T_c is finite.* In this regime one observes the critical behavior of the classical (thermal) transition.

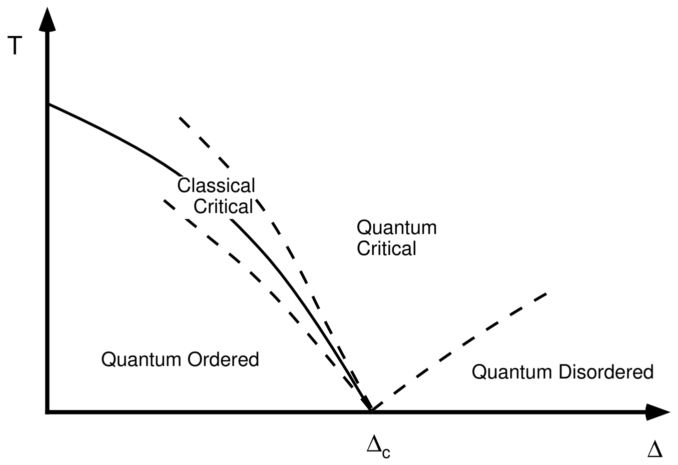

FIG. 1. A sketch of the various regions which occur when a parameter Δ drives T_c to zero. The phase boundary is indicated by the solid line. The dashed lines indicate regions where crossovers occur between different types of behavior. The region of classical critical behavior shrinks to zero as $T_c \to 0$. The quantum universality class is obtained as one goes through the quantum critical point at $T = 0, \Delta = \Delta_c$ from the quantum disordered to the quantum ordered regime.

Note, however, that the lower is T_c, the closer to criticality one has to be to observe classical critical behavior. If T_c is forced to zero by changing some parameter in the Hamiltonian, and the transition at $T = 0$ is traversed by changing this parameter, then one is *never* in the classical regime. Instead, one observes critical behavior of a *quantum universality class* which is different, in general from the *classical universality class* of the finite T_c transition. Fig. 1 sketches a typical phase diagram [1], in which Δ denotes the parameter which drives T_c to zero. One sees that the regime of classical critical behavior shrinks to zero as $T_c \to 0$. The new quantum universality class is observed in the quantum disordered and quantum ordered regimes. In the intermediate regime (sometimes called the quantum critical regime) the only energy scale is $k_B T$ and the there are interesting predictions [1,3] for the dynamical scaling functions which turn out to depend only on the ratio $\hbar\omega/k_B T$. I shall not, however, discuss this regime here.

It is well known [1,4] that the quantum problem can be described in terms of an effective classical action in d space plus one imaginary time dimensions. The size of the system in the imaginary time direction is $\hbar/k_B T$. In this picture it is easy to see why quantum mechanics is only important at $T = 0$. At any finite temperature we are dealing with a slab, infinite in the space directions but finite in the time direction. When the correlation "length" in the time direction reaches the thickness of the slab, the growth of correlations with time becomes limited by the slab thickness, and can be described by the techniques of finite size scaling [5]. The critical behavior is then just controlled by the diverging correlation length in the space directions, *i.e.* we have a d-dimensional classical problem. However, when T is zero, the size of the system in the time direction is infinite, just as it is in the space directions, so we have to study a d+1 dimensional problem, which will generally have different critical behavior from that of the d-dimensional model. Thus the quantum to classical crossover is similar to a dimensional crossover. Note that for systems with quenched disorder, the disorder is independent of (imaginary) time and so is *perfectly correlated* in the time direction.

In simple cases of magnetic transitions, and with no disorder, one ends up with a classical model in one higher dimension [6], in which space and time are equivalent. Another way of saying this is that the dynamical exponent, z, is equal to one. However, in the cases of greatest interest, *i.e.* those with quenched disorder, space and time are *not* equivalent, so usually $z \neq 1$. This complicates the analysis of numerical data because scaling is *anisotropic*. Data analysis then has to be done using anisotropic finite-size scaling, see *e.g.* [7,8].

Quantum phase transitions with disorder are poorly understood because many of the standard techniques which work well for conventional finite-T transitions do not work in this case. For example, the perturbative renormalization group (ϵ-expansion) has been remarkably successful in elucidating the various universality classes of classical transitions at finite temperature, as well as giving precise estimates for critical exponents in many cases. However, applying the same approach here, the coupling constant describing the disorder grows to a large value as soon as it becomes relevant, rather than approaching a value of order ϵ. Hence the perturbation approach breaks down and there is a "flow to strong coupling". However, one approach which can still be used, at least in the cases studied here, is Monte Carlo simulations, and I shall describe below some results using the technique.

Just as the simplest model with a classical phase transition is the Ising model, the simplest random model with a quantum transition is arguably the Ising model in a transverse field whose Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x \ . \tag{4}$$

Here the $\{\sigma_i^\alpha\}$ are Pauli spin matrices, and the nearest neighbor interactions J_{ij} and transverse fields h_i are both independent random variables. We take all the J_{ij} to be positive, so the model is a ferromagnet, not a spin glass. The rest of this talk will focus on this model.

One interesting aspect of disordered systems is that they have singularities away from the critical point, which have no counterpart in pure systems. These effects, called Griffiths singularities [9], are rather weak at thermal (finite-T) transitions but can give surprising and spectacular effects in the quantum case.

We will illustrate this physics for the transverse field Ising model described above. Let us assume that the system is in the paramagnetic phase at very low temperature. Due to fluctuations in the strength of the random bonds and transverse fields, there will be local regions where the bonds are stronger than average and the fields weaker than average such that this region is "locally in the ferromagnetic phase". The probability of this occurring is exponentially small in the volume v of the region, i.e. $\exp(-a\,v)$, where a is a constant. The spins in the region will be very strongly correlated and will flip as a coherent unit over a very long time scale which is exponentially large in the volume, i.e. $\exp(c\,v)$, where c is another constant. A simple change of variables indicates that there is a power law, rather than an exponential distribution of local relaxation times [10].

This leads to power law decay of the average time-dependent correlation functions, and power law variation of the susceptibility with T, i.e. $\chi \sim T^{\mu}$, where the exponent μ is expected to vary with as one moves along the horizontal axis (in the paramagnetic phase, i.e. $\Delta > \Delta_G$) in Fig. 1, where Δ here represents the ratio of the average value of h to the average of J. In certain cases it is possible that μ might be negative (so χ diverges as $T \to 0$) for a range of values Δ for $\Delta > \Delta_c$. This certainly happens in 1D [11], as was first found, though not the current understanding of it, by McCoy [12], who studied the two-dimensional *classical* Ising model with correlated disorder, which corresponds to the quantum transition in the 1D transverse field Ising model with point disorder. One of the goals of my work has been to try to see if this surprising result is special to one-dimension or whether it is also true in higher dimensions.

D. Fisher [11] has obtained many exact results for the 1D random transverse field Ising model using an real space renormalization group method which is exact on large length scales. In one-dimension there is no ferromagnetic order at finite temperature, so the phase boundary in Fig. 1 is squashed down to the $T = 0$ axis, but, along the $T = 0$ line there is a region of ferromagnetic order for $\Delta < \Delta_c$ which gives rise to paramagnetism for $\Delta > \Delta_c$.

Among the surprising results found by Fisher are:

1. The σ^z–σ^z correlation functions have such a very broad distribution that the average and typical [13] values behave differently. In the disordered phase at $T = 0$ the correlation length of the average correlation function diverges as $\Delta \to \Delta_c$ with an exponent $\nu_{av} = 2$, while the typical correlation length has an exponent $\nu_{typ} = 1$.

2. At the quantum critical point, the average correlation function decays with distance r with a power law, $r^{-\lambda}$, where λ is an irrational number, $\lambda = (3 - \sqrt{2})/2 \simeq 0.38$. However, the typical correlation function decays with a stretched exponential function, $\exp(-cr^{\sigma})$ where $\sigma = 1/2$.

3. The dynamical critical exponent, z is infinite. Rather than the characteristic time scale, τ, varying with a characteristic length scale ξ like $\tau \sim \xi^z$ as usual (which is known as "conventional dynamical scaling") one has $\ln \tau \sim \xi^{\psi}$ (with $\psi = 1/2$), which is known as "activated dynamical scaling".

In one-dimension, not only can many results be obtained analytically, but there is also an elegant numerical approach, using a mapping to free fermions [16,17], which can give numerically exact results for samples of order a thousand spins or so. This has been used to confirm the analytical results and also extend them to obtain information on entire distributions of correlation functions, and finite-temperature and dynamical properties [17,15].

An important question is whether these striking results are a special feature of 1D, or whether they are valid more generally. Unfortunately, the analytical approach is only valid in 1D, and very little is known in higher dimensions. Also the mapping to free fermions is also only valid in one-dimension. Hence, to obtain quantitative information for $d > 1$ we have used quantum Monte Carlo simulations [18].

We used the path integral representation in which the model is represented in d space (we just took $d = 2$) and one (imaginary time) direction. Time, like space, is discretized, and standard manipulations show that one has a $(d+1)$–dimensional Ising model, with disorder perfectly correlated in the time direction, as mentioned above.

The main technical difficulty is that the model is anisotropic, due to the correlated disorder. Hence the range of correlations in the time direction, τ is not equal to the range in the space directions, but (for a bulk system and assuming for now conventional dynamical scaling) these are related by $\tau \sim \xi^z$. In order to extrapolate data from finite sizes to the thermodynamic limit one uses the technique of finite-size scaling [5]. Here, one needs to generalize finite-size scaling to the anisotropic case. If the system is of size L in the time direction, and L_τ in the time direction, then one needs to let both L and L_τ tend to infinity but with the ratio L_τ/L^z, called the aspect ratio, fixed [7,8]. The problem, then, is that to do the simulations one needs to already know z in order to choose appropriate sizes, but one does not know z until the simulations have been carried out. In practice, one has to scan a range of values of both L and L_τ and find a systematic method of both locating the critical point and determining z.

The main conclusions from Ref. [18], which just studied 2D, are that the behavior is similar to that in 1D, though with different values for the exponents. More precisely we find:

1. There is evidence, which is quite good but not totally compelling, that one has acti-

vated, rather than conventional, dynamical scaling at the critical point.

2. There is very solid evidence that whereas the average correlation function at the critical point falls off with a power of r, the typical correlation function falls off much faster, consistent with a stretched exponential.

Attempts were also made to look at the correlations away from the critical point to see if the correlation length exponents for average and typical correlations are different. Although there is evidence that this is the case, the results were not entirely consistent and so cannot be considered conclusive.

More recently, Mau et al. [19] have looked at the 2D random transverse field Ising model by implementing numerically the real space renormalization group approach that was studied analytically in 1D by Fisher [11]. Their results indicate that the same type of "infinite-randomness quantum fixed point" applies in 2D as well as in 1D, in agreement with our [18] conclusions. In addition Mau et al. were able to get a good estimate of the correlation length exponents.

To conclude, we have seen that the behavior of a disordered system near a quantum phase transition is very unusual, at least if there is discrete (Ising) symmetry. There are strong Griffiths-McCoy singularities (and possibly divergences), even in the paramagnetic phase, and unusual critical phenomena. It would be interesting to try to see these effects experimentally.

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