Numerical Simulations of Quantum Phase Transitions

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Abstract

In this talk I will describe some examples of quantum phase transitions with disorder and explain in what ways these transitions differ from conventional phase transitions at finite temperature. It will be explained that the ϵ-expansion does not work and so much of what we know has come from numerical simulations. A novel feature is the importance of "Griffiths singularities", which come from rare, strongly correlated, regions of the system. Some recent results on the quantum spin glass will be discussed in a little more detail.

1 Introduction

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.

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 [1] to define a dynamical exponent, z, by

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

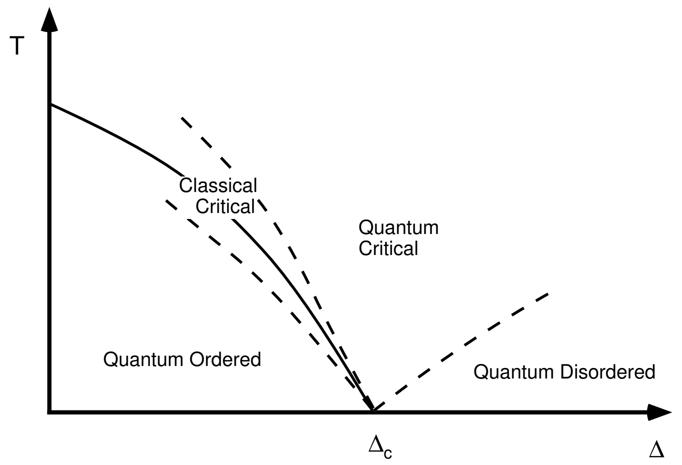

Figure 1: A sketch of the various regions which occur when a parameter Δ drives T_c to zero. The phase boundary is indicated by the solid line. The dashed lines indicate regions where crossovers occur between different types of behavior. The region of classical critical behavior shrinks to zero as $T_c \to 0$. 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.

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.

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 [2], 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 [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 [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, 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].

In the rest of this talk I will give some examples of quantum phase transitions with disorder, discuss what new physics arises in these systems, and summarize why this is rather poorly understood. Because analytical work has proved hard, much of what we know has come from simulations. I will discuss briefly some of the recent numerical work on a particular problem, the quantum spin glass.

2 Examples

The most commonly studied quantum phase transition is the metal-insulator transition [9]. In a disordered system, some or all of the electron states are *localized*, *i.e.* they have a finite amplitude to be on a site in a particular region of the lattice, and negligible amplitude to be outside this region. If the Fermi energy lies in a region of localized states, the system is an insulator. (At finite temperature however, conduction can occur because *inelastic* scattering processes, *e.g.* due to phonons, can kick an electron from one localized state to another.) In three and more dimensions, and for weak disorder, only the states at the edge of the band are localized, and there is a "mobility edge" separating these states from extended states at the center. If the degree of disorder, or the density of electrons, is changed, the Fermi energy can go from being in a region of extended states to a region of localized states: this is the metal-insulator transition. At a critical value of disorder, *all* the states become localized. It turns out that in two dimensions, all states are localized for *any* non-zero disorder, *i.e.* the critical value of disorder is zero.

Denoting by δ the deviation from criticality then the $T = 0$ conductivity is found to vanish on the metallic side like

$$\sigma \sim \delta^{\mu} , \tag{4}$$

and, of course, to be identically zero on the insulating side. One goal of theory is to calculate the exponent μ and compare with experiment. Numerical work [10] finds $\mu \simeq 1.4$ and the experimental values [10] range from about this down to much lower values. This wide range reflects the difficulty of extrapolating the data to $T = 0$ and possibly also indicates a rather narrow critical region (the region in which asymptotic scaling behavior is seen).

Analytical work has been developed for this model, based on a $2+\epsilon$ expansion [11], but this does not seem to converge well in $d = 3$. Unfortunately, there is no expansion away from an upper critical dimension (which, in the case of classical critical phenomena, is better behaved), and it is not known whether an upper critical dimension (above which the exponents would stick at some "mean field" value) even exists.

One difficulty with the metal-insulator transition is that there is no obvious order parameter. This is not the case for my second example, the superconductor-insulator transition in disordered thin films. I have already mentioned that there is no metallic state at $T = 0$ in a two-dimensional system with disorder because all the electron states are localized. However, superconductivity (which involves a coherent propagation of a *pair* of electrons) is not ruled out, though it too will presumably be eliminated if the disorder is strong enough. In 2-d one therefore has the possibility of a direct transition from a superconductor to an insulator without going through an intervening metallic phase, as one changes the degree of disorder. The order parameter is just the amplitude of the pair condensate, as usual in a superconducting transition, and so one can formulate standard methods, such as Ginzburg-Landau theory.

An interesting prediction [12] is that the system *is* metallic (*i.e.* has a finite conductivity) precisely *at* the critical point and that the value of the conductivity there, σ_c, is *universal.* To be more precise,

$$\sigma_c = C\sigma_Q , \tag{5}$$

where C is a universal constant and

$$\sigma_Q = \frac{(e^{\star})^2}{h} \tag{6}$$

is the quantum of conductance, with $e^{\star} = 2e$, the charge of a Cooper pair. A goal of the theory is to calculate this universal conductance as well as standard universal quantities such as critical exponents. Experimental estimates [13] of σ_c vary over a range of about a factor of three, which, if correct, would mean that σ_c is not universal after all, but it is possible that many of the experiments did not probe the asymptotic critical region, often very small in superconductors.

Although this model can be reformulated in a Ginzburg-Landau picture, an ϵ-expansion about an upper critical dimension does not work [14], since the renormalization group flows go to strong coupling. Since the analytic renormalization group approach doesn't work, much of what we know has been learned from Monte Carlo simulations, *e.g.* [7].

My third and final example of a quantum phase transition is a magnetic system. Suppose we have an Ising magnet, where the spins lie up or down. These are eigenstates of the Pauli spin matrix σ^z, so the Hamiltonian can be written as

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z \ . \tag{7}$$

We shall assume that the interactions J_{ij} are random and *frustrated*, *i.e.* have random signs so that no spin configuration simultaneously minimizes all the terms in the Hamiltonian. Such a system is called a *spin glass* [15]. Typically one chooses an Edwards-Anderson model, considering only nearest neighbor interactions which are independent random variables chosen from a symmetric distribution, *i.e.*

$$[J_{ij}]_{\rm av} = 0 \ ; \quad [J_{ij}^2]_{\rm av} = J^2 \ . \tag{8}$$

So far, all operators commute so one could just replace the spin operators by c-numbers, ± 1, which is the usual way to present the Ising model. Next, however, add a transverse field which couples to σ^x so the Hamiltonian becomes

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{i,j} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x \ . \tag{9}$$

The problem is now quantum mechanical since σ^x and σ^z don't commute. If the system has a finite-temperature transition with $\Gamma = 0$, then turning on Γ will decrease T_c since the transverse field cants the spins away from their ordering direction (the z-direction). If Γ is big enough, T_c can be depressed to zero and a quantum critical point results.

An experimental system for which Eq. (9) should be a good model has been studied in Ref. [16]. One advantage of this system is that one can tune through the quantum transition by varying the transverse field, a continuous parameter, whereas in the other systems I have mentioned one generally has to vary the degree of disorder, which cannot be changed continuously and for each data point one has to grow a new sample.

For the quantum spin glass, as for the other examples mentioned above, we do not have an ϵ-expansion away from an upper critical dimension [17], so the only estimates for critical exponents, at least for short range interactions, have come from Monte Carlo simulations [8, 18] on the model described by Eq. (9). These will be described in section 4.

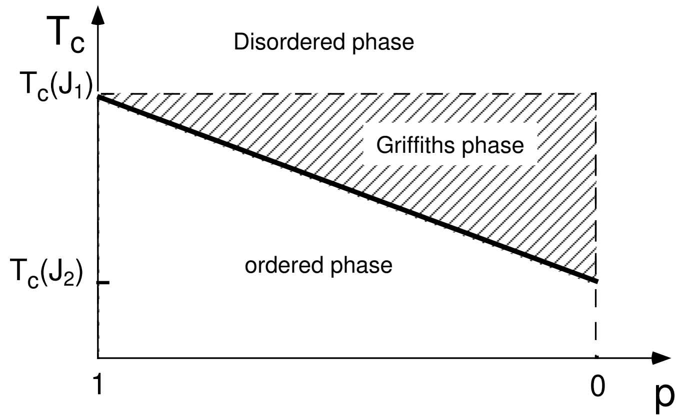

Figure 2: A sketch of the phase diagram of the model described by Eqs. (7) and (10), showing the Griffiths phase, where the free energy is a non-analytic function of magnetic field h. The phase boundary is indicated by the thick line. For this classical model the Griffiths singularity is an essential singularity, *i.e.* very weak. However, the corresponding singularity is much stronger for quantum transitions at $T = 0$.

3 Griffiths Singularities

In this section I will discuss an aspect of phase transitions in disordered systems which has no counterpart in pure systems. These effects, called Griffiths singularities [19], are rather weak at thermal phase transitions but can give surprising and spectacular effects in the quantum case.

To illustrate Griffiths singularities, consider first a simple *classical* spin model, as in Eq. (7), where the interaction can take one of two values, *i.e.*

$$J_{ij} = \begin{cases} J_1 & \text{prob. } p \\ J_2 & \text{prob. } 1-p \end{cases} \tag{10}$$

Assume that J_1 and J_2 are both positive, so there is no frustration, and $J_1 > J_2$. The resulting phase diagram is sketched in Fig. 2. The Griffiths phase is the region which would be below T_c if all the interactions had their largest possible value (J_1 in this case) but is actually above the T_c of the random system. Griffiths singularities arise in the Griffiths phase because there is a probability of having a large region with all J_1 bonds which would be locally ordered. Since an ordered system has a large response to a magnetic field, h, the free energy turns out not to be an analytic function of h at $h = 0$ in the Griffiths phase [19]. The probability of having a large region with all J_1 bonds is exponentially small, and, as a result, the singularity is very weak at a thermal transition, just an essential singularity [20]: all derivatives of the free energy with respect to h are finite.

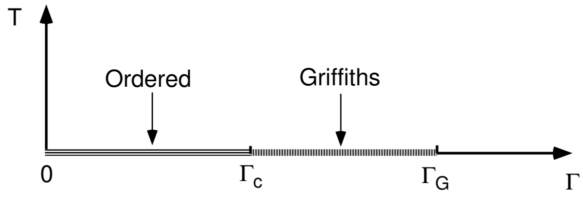

Figure 3: A sketch of the phase diagram of the one dimensional random transverse Ising model. The ordered phase only occurs at $T = 0$. In the Griffiths phase the free energy is a non-analytic function of magnetic field h, the singular part varying as in Eq. (11), where δ is a function of Γ tending to unity as $\Gamma \to \Gamma_c^+$ and tending to infinity as $\Gamma \to \Gamma_G^-$.

Although the effects of Griffiths singularities on static properties are probably unobservably weak for thermal transitions, they have a much bigger effect on quantum transitions. For the one dimensional version of the quantum spin glass model of Eq. (9) these can be worked out in detail and are quite spectacular. This was first studied by McCoy and Wu [21] in the equivalent (1+1)-dimensional classical version, an Ising model with disorder which is perfectly correlated along one direction. Subsequently, new results and a great deal of insight were obtained by Fisher [22]. A one-dimensional system with short range interactions has no long range order except at $T = 0$, so the ordered region is entirely along the Γ axis, as shown in Fig. 3. The system is ordered up to a critical value Γ_c. However, there is a finite region in the disordered phase, $\Gamma > \Gamma_c$ where the susceptibility is infinite. This is most unusual because the susceptibility normally diverges *at* the critical point. In fact the free energy is a non-analytic function of field, h, in the disordered region, up to $\Gamma = \Gamma_G$, the end of the Griffiths phase. Γ_G is the value Γ_c would have if all the interactions had their largest value. Unlike the essential singularity in the case of thermal transitions, one has a much stronger effect here:

$$f_{sing} \sim |h|^{\delta(\Gamma)} , \tag{11}$$

where δ is a function of Γ tending to unity as $\Gamma \to \Gamma_c^+$ and tending to infinity as $\Gamma \to \Gamma_G^-$. The value of Γ at which the susceptibility diverges is now seen to have no special significance, but is just the point where $\delta = 2$. Griffiths singularities also give striking effects in the dynamics. The dynamical exponent varies continuously in the Griffiths phase and *diverges* at the critical point [22]. This has recently been confirmed in numerical studies [23] using the representation of the problem in terms of non-interacting fermions [24].

These results occur because of rare regions which are more strongly correlated than average and are locally in the ordered phase. A rough argument, which applies for arbitrary d, goes as follows: The probability of finding a region of volume L^d which is locally in the ordered phase is of order

$$P(L) \sim e^{-\mu L^d} , \tag{12}$$

where μ is some constant. Consider now the spins as a function of (imaginary) time in this region. To change the sign of the magnetization requires inserting a domain wall, whose energy is σL^d, where σ is the surface tension. Hence the relaxation time in this region is of order

$$\tau \sim e^{\sigma L^d} \ . \tag{13}$$

In other words, there is an exponentially small probability of having an exponentially large relaxation time. Consequently the distribution of relaxation times follows a power law,

$$P(\tau) \sim \frac{1}{\tau^{1+\frac{\mu}{\sigma}}} \ , \tag{14}$$

as does the local time dependent spin-spin correlation function,

$$\langle \sigma_i^z(t)\sigma_i^z(0)\rangle \sim \frac{1}{t^{\frac{\mu}{\sigma}}} \ , \tag{15}$$

where t is imaginary time. The local susceptibility is obtained by integrating over t and so diverges if $\mu/\sigma < 1$.

This argument, while crude, suggests that the form of the singularity in Eq. (11) should apply quite generally to the Griffiths phase at $T = 0$ in Ising systems, though the dependence of δ on Γ presumably depends on the model. In particular, it is not clear whether the susceptibility will diverge in the Griffiths phase except in $d = 1$. It is in part to try to answer this question that numerical work on the quantum spin glass Ising Hamiltonian in Eq. (9) has been undertaken [8, 18]. This will be described in the next section.

4 Ising Spin Glass in a Transverse Field

Recently large scale simulations have been carried out on the quantum spin glass Hamiltonian in Eq. (9), both in two [8] and three [18] dimensions. As described in those references, the simulation involves an effective classical action in d spin plus one imaginary time dimensions. The interactions in the space directions have a Gaussian distribution with zero mean and standard deviation of unity and are *independent* of imaginary time, while the interactions between the "time slices" are ferromagnetic and all equal to unity. Increasing the effective temperature in the classical action disorders the system and so corresponds to increasing the strength of the transverse fields.

The system in (9) is very anisotropic, so, according to a finite size scaling hypothesis [5] extended to anisotropic systems [25], thermodynamic quantities close to the critical point depend on *two* independent scaling variables, which we can take to be $\delta L^{1/\nu}$ and the aspect ratio L_τ/L^z. The scaling analysis is straightforward only if it depends on a single parameter, so it is necessary to fix the aspect ratio. Since z is unknown, one has to scan several different sample shapes to see which choice for z scales best.

As in standard spin–glass theory [15], we define the overlap between the configurations of two replicas, 1 and 2, with the same disorder as

$$Q = \frac{1}{L^d L_\tau} \sum_{i,\tau} S_i^{(1)}(\tau) S_i^{(2)}(\tau) \quad , \tag{16}$$

and for each disorder realization we calculate the dimensionless combination of moments

$$g = 0.5\Big[3 - \langle Q^4\rangle / \langle Q^2\rangle^2\Big] \quad . \tag{17}$$

The disorder averaged quantity, $g_{\rm av} = [g]_{\rm av}$ obeys the finite size scaling form

$$g_{\rm av}(K, L, L_\tau) = \tilde{g}_{\rm av}(\ \delta L^{1/\nu},\ L_\tau / L^z\ )\ , \tag{18}$$

and has the property [26] that it vanishes in the disordered phase for $L \to \infty$, and tends to a finite value in the ordered phase. Consequently, $\tilde{g}(x, y)$ vanishes at fixed x both for $y \to 0$ (where the system is a classical two–dimensional spin glass at finite "temperature", which is disordered) as well as for $y \to \infty$ (where the system is effectively a long one–dimensional chain along the τ direction, which is also disordered). Hence, $\tilde{g}(x, y)$ must have a maximum at some value of y for fixed x. We used this to estimate the "temperature" of the effective classical action which we find is given by $T_c^{cl} = 3.275 \pm 0.025$. Furthermore, at the critical point, the values of L and L_τ for which $\tilde{g}$ is a maximum are related by $L_\tau \sim L^z$. By this method we determine the dynamical exponent and get $z = 1.50 \pm 0.05$.

One can also calculate the non-linear susceptibility, which is measured in experiments. Results for the dependence of χ_{nl} on L at the critical point in Fig. 4 show that this divergenes as $L^{4.7}$, which, using finite-size scaling, translates into a divergence with L_τ ($\propto 1/T$) at fixed L of $L_\tau^{4.7/z}$. Using $z \simeq 1.5$ this leads to the prediction that the non-linear susceptibility at the critical value of Γ should diverge roughly like $1/T^3$. A similar strong divergence is also found in 3-d [18]. The reason for the discrepancy with experiment [16], where only a weak divergence was found, is unclear.

Recent studies have also been carried out [27] in the disordered phase of the 2-d model to look at Griffiths singularities. The distributions of the local susceptibility and local non-linear susceptibility (i.e. the non-linear response of a spin on site i to a field on that site) show power law tails as expected from Eq. (14). The power decreases (showing that there are more long relaxation times) as one approaches the critical point. However, the effects of Griffiths singularities are less spectacular than in 1-d. For example, the dynamical exponent is finite at the critical point, as already noted above. Whereas in 1-d Griffiths singularities seem to control the critical behavior, in 2-d they seem to ride along on top of the critical behavior and simply contribute additional singularities in the scaling functions in the limit $L_\tau / L^z \to \infty$.

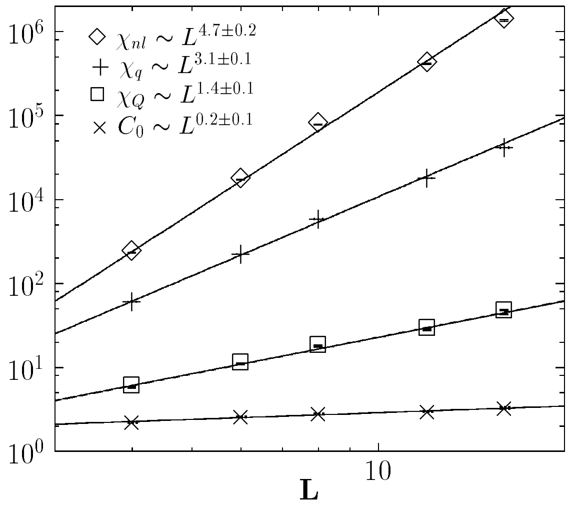

Figure 4: The diamonds show the non-linear susceptibility as a function of system size at the critical point, $T^{cl} = 3.30 \simeq T_c^{cl}$, on a double logarithmic plot. The slope is about 4.7, indicating a strong divergence. From ref. [8].

5 Conclusions

The physics of quantum phase transitions with disorder remains poorly understood compared with our rather complete understanding of thermal phase transitions. We have seen that non-perturbative effects (Griffiths singularities) have a significant effect, especially in one-dimension. The simulations seem of the critical behavior of the quantum spin glass seem to be under fairly good control, but indicate a large divergence in the non-linear susceptibility, in contrast to experiments. This discrepancy remains to be understood.

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