

# QUANTUM SPIN GLASSES

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**Abstract.** Ising spin glasses in a transverse field exhibit a zero temperature quantum phase transition, which is driven by quantum rather than thermal fluctuations. They constitute a universality class that is significantly different from the classical, thermal phase transitions. Most interestingly close to the transition in finite dimensions a quantum Griffiths phase leads to drastic consequences for various physical quantities: for instance diverging magnetic susceptibilities are observable over a whole range of transverse field values in the disordered phase.

## 1 Introduction

At very low temperatures the role of quantum fluctuations in any physical pure or disordered system become more and more important. As far as critical phenomena are concerned any finite temperature destroys quantum coherence of the lowest lying excitations determining the universality class of the transition, which remains therefore classical. However, if the transition takes place at strictly zero temperature, a new universality class and in particular new physics emerges. Obviously in the vicinity of such a transition even finite temperature properties are characterized by strong crossover effects between a quantum critical and classical regions. Thus the properties of such zero temperature transitions become experimentally accessible, which motivates the study these new universality classes.

The prominent feature of quantum phase transitions [1] is the fact that statics and dynamics are inextricably linked: the static features are defined by the Hamiltonian, which implies immediately the dynamics via the Schrödinger equation. This introduces an extra dimension, the (imaginary) time, into the problem and it is by no means guaranteed that this additional dimension is equivalent to one of the  $d$  space dimensions. In many *pure* systems it turns out to be so, which is the origin of the observation that “the correlation length is proportional to the inverse energy gap”. This relation seems to be pretty robust even in the presence of a nontrivial anisotropy (c.f. the ANNNI model), for which reason it became folklore in strongly correlated systems.

However, in the presence of quenched (i.e. time-independent) *disorder*, this simple relation fails: Usually the randomness (modeling impurities etc.) is uncorrelated in space, but time-independence means a perfect correlation of the disorder in the time direction. This implies an *extreme* anisotropy, which manifests itself in a non-trivial relation between spatial correlation length  $\xi$

and energy gap  $\Delta E$ . For a generic second order phase transition scenario a dynamical exponent  $z$  can be introduced via  $\xi \sim \Delta E^{-z}$ , with  $z$  in general different from one.

Another drastic consequence of the perfect correlation of the disorder in the (imaginary) time direction are spectacular properties of physical observables within the so called Griffiths phase [2] surrounding the critical point itself. In contrast to the classical case one there may be a whole region of values for the parameter tuning the transition over which the zero-frequency susceptibilities *diverge*. Such a scenario has actually been described already a long time ago by McCoy [3] in the context of a one-dimensional model. It seems that this is indeed a generic feature of finite dimensional disordered systems with a quantum phase transition as we would like to demonstrate here.

In this article we focus on quantum spin glasses, in particular the transverse field Ising models defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x, \quad (1)$$

where  $\sigma_i$  are the Pauli spin matrices (modeling spin- $\frac{1}{2}$  degrees of freedom),  $\langle ij \rangle$  nearest neighbor pairs on a  $d$ -dimensional lattice,  $\Gamma$  the transverse field and  $J_{ij}$  quenched random interaction strength obeying for instance a Gaussian distribution with zero mean and variance one. Here the quenched disorder mentioned above also produces frustration, which enhances the effect that the randomness has on critical and non-critical properties. For completeness we also include a discussion of the one-dimensional case, which is not frustrated but shares many features of the higher dimensional realizations. In the next section we report on the results for the critical properties and in section 3 we present the exciting features of the Griffiths phase in these models. Section 4 gives a summary and perspectives for future work.

## 2 Critical Properties

In any dimension  $d$  the quantum system described by eq. (1) has a second order phase transition at zero temperature that manifests itself in specific macroscopic properties of the ground state and low lying excitations. A critical value  $\Gamma_c$  for the transverse field strength separates a disordered or paramagnetic phase for  $\Gamma > \Gamma_c$  from an ordered phase for  $\Gamma < \Gamma_c$ . This transition is characterized by a diverging length scale  $\xi \sim |\Gamma - \Gamma_c|^{-\nu}$  and a vanishing characteristic frequency  $\omega \sim \Delta E \sim \xi^{-z}$ . The latter is the quantum analog of “critical slowing down” in the critical dynamics of classical, thermally driven transitions. Together with a third critical exponent, defining the anomalous dimension of the order parameter field, the thermal exponent  $\nu$  and the dynamical exponent  $z$  give a complete description of the transition via a set of scaling relations for two and three dimensions. The one-dimensional case

shows a somewhat richer scenario [4] and in  $d > 8$  the violation of hyper-scaling adds another exponent [5]. We list the main features for the different dimensions:

## 2.1 $d=1$

Analytical [3], [4] and numerical [6], [7] investigations revealed the following picture: because of the logarithmically broad distribution of various physical quantities at criticality one is forced discriminate between average and typical properties. For instance the typical correlation length diverges with an exponent  $\nu_{\text{typ}} = 1$ , whereas the average diverges with  $\nu_{\text{av}} = 2$ . It turns out that it is not the energy gap but its logarithm that scales with system size and distance from the critical point, giving rise to an exponential rather than algebraic decrease of the energy gap with system size:  $[\Delta E]_{\text{av}} \sim \exp(-aL^{1/2})$ . This means that  $z = \infty$  and since the inverse gap corresponds to a characteristic relaxation or tunneling time it is reminiscent of an activated dynamics scenario in conventional spin glasses or random field systems.

For numerical work with finite size systems it is most useful to study the probability distribution of various quantities, such as the energy gap or local susceptibility  $\chi^{(\text{loc})}(\omega = 0)$ . One finds at the critical point

$$P_L(\ln \chi^{(\text{loc})}) \sim \tilde{P}(L^{-1/2} \ln \chi^{(\text{loc})}) \quad (2)$$

reflecting both features  $\nu_{\text{av}} = 2$  (since the system size enters with a power  $1/\nu_{\text{av}}$ ) and  $z = \infty$  (since  $\ln \chi^{(\text{loc})}$  rather than  $\chi^{(\text{loc})}$  enters the scaling variable).

## 2.2 $d = 2$ and $3$

Numerical investigation of the two- [8] and three-dimensional [9] quantum Ising spin glass model in a transverse field via quantum Monte Carlo simulations demonstrated the existence of a second order phase transition at a critical transverse field strength  $\Gamma_c$ . The results are compatible with the scaling predictions made by a droplet theory for these models [10].

In contrast to the one-dimensional case there is ample evidence that here the dynamical exponent  $z$  is finite, namely  $z = 1.50 \pm 0.05$  in two and  $z = 1.3 \pm 0.1$  in three dimensions. Also the subsequent study [11, [12] of the probability distribution of the logarithms of the local linear and nonlinear susceptibility at criticality gave no indication of a characteristic broadening with increasing system size that would indicate an infinite value for  $z$ .

Most interestingly, as mentioned in the introduction, the critical exponents for the quantum phase transition at strictly zero temperature are connected to the temperature dependence of various quantities for  $\Gamma = \Gamma_c$ ,

$T \rightarrow 0$ . For instance the experimentally accessible nonlinear susceptibility *diverges* at  $T = T_c$  quite strongly, i.e.

$$\chi_{\text{nl}}(\omega = 0) = \left. \frac{\partial^3 M}{\partial h^3} \right|_{h=0} \propto T^{-\gamma_{\text{nl}}/z} \quad (3)$$

with  $\gamma_{\text{nl}}/z \approx 3.0$  in two and in three dimensions ( $M$  is the total magnetization and  $h$  a longitudinal magnetic field). Thus the strength of the divergence of the non-linear susceptibility is similar to the one at the classical transition. This is in sharp contrast to the results reported for recent experiments on  $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$  [13]. Here the strength of the divergence seemed to decrease with decreasing temperature, and it has been speculated that at zero temperature, i.e. at the quantum phase transition, no divergence at all might be present (see next subsection). On the other hand, it might be possible that because of the long range nature of the dipolar interactions in  $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$  the experiments might be better described by a model with appropriately chosen long range interactions.

### 2.3 Mean field ( $d=\infty$ )

The quantum phase transition occurring in the infinite range model of the transverse Ising spin glass [14] and in a related quantum rotor spin glass [15], [5] can be handled analytically to a large extent [16]. The dynamical exponent is  $z = 2$ , the correlation length exponent  $\nu = 1/4$  and the nonlinear susceptibility diverges with an exponent  $\gamma = 1/2$ . The latter again implies a divergence of the non-linear susceptibility. Although it is much weaker than for short range interaction models it should clearly be observable. However, the experiments [13] at small but finite temperatures yield an effective exponent  $\gamma_{\text{eff}}$  that is significantly smaller than  $1/2$ , and for  $T < 25$  mK even one that is indistinguishable from zero. Therefore also mean-field theory does not cure the contradiction between experiment and theory for transverse Ising spin glasses.

Finally we would like to remark that the zero temperature phase transition in a number of mean field quantum spin glasses falling in universality classes different from the one considered here has been investigated recently [17].

## 3 Griffiths Phase

In a specific disorder realization one can always identify spatial regions that are more weakly or more strongly coupled than the average. The latter lead to a non-analytic behavior of the free energy not only at the critical point but in a whole region surrounding it, as already observed by Griffiths nearly 30 years ago [2]. However, a strongly coupled cluster (in spin glass terms one with a minor degree of frustration) tends to order locally much earlier,

coming from the disordered phase, than the rest of the system. Upon application of an external field spins in this cluster act collectively and thus lead locally to a greatly enhanced susceptibility. However, one only gets an essential singularity in static properties of a classical system [2].

This effect is much stronger in dynamics than in statics. For classical disordered Ising system with heat bath dynamics close to a thermally driven phase transition it was shown [18] that these strongly coupled regions possess very large relaxation times for spin autocorrelations. By averaging over all sites one gets a so called enhanced power law

$$C_{\text{classical}}(t) = [\langle S_i(t)S_i(0) \rangle]_{\text{av}} \sim \exp\left\{-a(\ln t)^{d/d-1}\right\} \quad (4)$$

where  $[\dots]_{\text{av}}$  means an average over all sites and disorder realizations. However, this prediction, although rigorous to some extent (at least for the diluted ferromagnet [19]), could not be confirmed by extensive numerical investigations, neither for the spin glass [20] nor for the diluted ferromagnet [21], [22]. The main reason for this failure is most probably the extremely small probability with which big enough strongly coupled clusters that have an extremely large relaxation time occur in a finite size systems [22].

To make this point clear let us focus, for simplicity, on a diluted Ising ferromagnet below the percolation threshold, i.e. the site concentration  $c < p_c$ . Then a connected cluster of volume  $V = L^d$  occurs with a probability  $p = c^V = \exp(-\zeta L^d)$  with  $\zeta = \ln 1/c > 0$ , which is a very small number for large  $L$ . However, these spins within this cluster have a relaxation time  $\tau$  that is exponentially large (because of the activation energy that is needed to pull a domain wall through the cluster to turn it over):  $\tau \sim \exp(\sigma L^{d-1})$ , with  $\sigma$  a surface tension. The combination of these two exponentials yield the result (4). Note that the occurrence of the exponent  $d - 1$  in the relaxation time renders the final decay of the autocorrelation function *faster* than algebraic.

This is quite different in a random quantum system at zero temperature. Now the activated dynamics in the classical scenario has to be replaced by tunneling events. Let us stick to the above example of a diluted ferromagnet and add a transverse field at zero temperature. The probability for a connected cluster to occur is the same as before, but the relaxation time or inverse tunneling rate is now given by  $\tau \sim \exp(\sigma' L^d)$ . Remember that the classical ground state of the cluster under consideration would be ferromagnetic and twofold degenerate. The transverse field lifts this degeneracy for a finite cluster, but for  $T$  smaller than the critical field value, where the ferromagnetic order of the infinite pure system sets in, the energy gap is extremely small: it decreases exponentially with the volume of the cluster. This energy gap between ground state and first excited state sets the scale for the tunneling rate.

Now we see that in marked contrast to the classical system a  $d$  instead a  $d - 1$  appears in the exponent for the relaxation time. One might say that the same cluster relaxes faster via activated dynamics (although that is already

incredibly slow) than by quantum tunneling. Therefore, by the same line of arguments that lead to (4), one now expects spin-autocorrelations to decay *algebraically* in the Griffiths phase of random quantum systems:

$$C_{\text{quantum}}(t) = \langle 0 | \sigma_i^z(t) \sigma_i^z(0) | 0 \rangle \sim t^{-\zeta(\Gamma)/\sigma'(\Gamma)} \quad (5)$$

For simplicity, although we expect a similar form for real time correlations, we assume  $t$  to be imaginary time, i.e. the Operator  $\sigma_i^z(t)$  to be given by  $\exp(-Ht) \sigma_i^z \exp(Ht)$ ,  $H$  being the Hamiltonian. Apart from a different functional form (5) has drastic consequences for various quantities: For instance the local zero frequency susceptibility at temperature  $T$  is given by

$$\chi^{(\text{loc})}(\omega = 0) = \int_0^{1/T} dt \langle C(t) \rangle \sim T^{-1+\zeta(\Gamma)/\sigma'(\Gamma)} \quad (6)$$

which *diverges* for  $T \rightarrow 0$  if  $\zeta(\Gamma)/\sigma'(\Gamma) < 1$  even if one is not at the critical point! Such a prediction should be experimentally measurable.

It should be noted that a diverging (surface) susceptibility in a whole region close to the critical point has already been found by McCoy nearly 30 years ago [3] for a classical two-dimensional Ising model with layered randomness, which is equivalent to the random transverse Ising chain. Actually we see now clearly that the non-analyticities reported by Griffiths [2] and the divergences calculated by McCoy [3] have a common origin: the existence of strongly coupled rare regions, which simply leads to a more drastic effect in a quantum system at low or vanishing temperatures than in a classical system.

### 3.1 $d = 1$

The random transverse Ising chain has been reinvestigated recently by D. Fisher [4] in a beautiful renormalization group treatment providing us with many astonishing analytical predictions. On the numerical side one can take advantage of the free fermion technique [23], by which the problem of diagonalizing the original quantum Hamiltonian is reduced to the diagonalization of a  $L \times L$  or  $2L \times 2L$  matrix. In this way one can consider very large system sizes ( $L \sim 256$ ) with good statistics (i.e. number of disorder realizations  $\geq 50,000$ ). However, we should note that some of the basic features of the model (e.g.  $z = \infty$  at criticality, existence of a Griffiths phase, etc.) can already be seen for modest system sizes ( $L \leq 16$ ) provided one studies the appropriate quantities which are sensible to the rare disorder configurations having strong couplings and/or small transverse fields. The probability distribution of the energy gap and/or various susceptibilities is such a quantity and in what follows we report the results of numerical investigations that support the above predictions.

In [7] we took a uniform distribution for bonds ( $J_i \in [0, 1]$ ) and transverse fields ( $h_i \in [0, h_0]$ ). The system is at its critical point for  $h_0 = 1$  (since in this case the field- and bond distributions are identical and therefore the

model self-dual) and in the paramagnetic (ferromagnetic) phase for  $h_0 > 1$  ( $h_0 < 1$ ). For each of 50,000 disorder realization for chains of length  $L$  (from  $L = 16$  to  $L = 128$ ) we calculated the energy gap  $\Delta$  from which we calculated the probability distribution  $P_L(\ln \Delta E)$ . It turned out that *at* the critical point  $h_0 = 1$  the probability distribution scales as described in section 2.1. according to eq. (2). In particular the distribution gets broader even on a logarithmic scale with increasing system size.

Within the Griffiths phase for  $h_0 > 1$ , however, the distribution does not broaden any more, but gets simply shifted on a logarithmic scale with increasing system size. It turns out that now the distribution of gaps obeys

$$\ln [P(\ln \Delta E)] = \frac{1}{z} \ln \Delta E + \text{const.} \quad (7)$$

with a dynamical exponent that varies continuously throughout the Griffiths phase according to  $1/z \sim 2\delta - c\delta^2$  ( $\delta$  being the distance from the critical point  $\delta = h - h_0$ ) and which diverges at the critical point  $z \rightarrow \infty$  for  $\delta \rightarrow 0$ . The form (7) can be made plausible by an argument applicable to any dimension  $d$  given in the next subsection.

### 3.2 $d = 2$ and $3$

For the numerical investigation of the astonishing features of the transverse field spin glass model defined in eq. (1) in 2 and 3 dimensions it is also most promising to focus on the probability distribution of the local linear and nonlinear susceptibility. The former is simply proportional to the inverse of the energy gap, whereas the latter is proportional to the third power of the inverse of the gap, hence the distribution of gaps  $P(\ln \Delta E)$  plays again the crucial role. The form that we expect is similar to (7) because of the following argument:

From what has been said in the beginning of section 3 before eq. (5), by combining the probability of a strongly coupled cluster with its energy gap one gets a power law for the tail of the distribution of gaps:  $P(\Delta E) \sim \Delta E^{\lambda-1}$  with  $\lambda = \zeta(I)/\sigma'(I)$ . Furthermore since the excitations that give rise to a small energy gap are well localized we assume that their probability is proportional to the spatial volume  $L^d$  of the system. Thus  $P_L(\ln \Delta E) \sim L^d \Delta E^\lambda$ , which can be cast into the conventional scaling form relating a time scale to a length scale via the introduction of a dynamical exponent:  $P_L(\ln \Delta E) \sim (L \Delta E^{1/z})^d$  with  $z = d/\lambda$ . Therefore the distribution for the local susceptibility (because  $\chi^{(\text{loc})} \propto 1/\Delta E$ ) should be given by

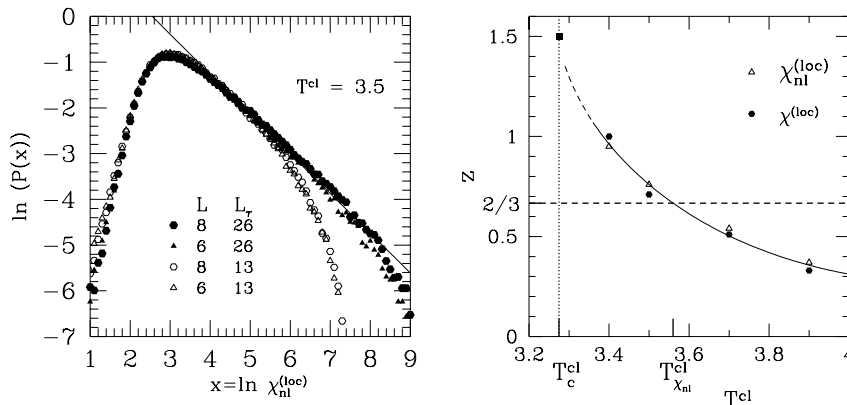
$$\ln [P(\ln \chi^{(\text{loc})})] = -\frac{d}{z} \ln \chi^{(\text{loc})} + \text{const.} \quad (8)$$

As a byproduct one obtains in this way also the form (7) for the one-dimensional case. The distribution of the local nonlinear susceptibility the

factor  $d/z$ , which is actually the power for the algebraically decaying tail of  $P(\chi^{(\text{loc})})$ , should be replaced by  $d/3z$  (since  $\chi_{\text{nl}}^{(\text{loc})} \propto 1/\Delta E^3$ ):

$$\ln \left[ P(\ln \chi_{\text{nl}}^{(\text{loc})}) \right] = -\frac{d}{3z} \ln \chi_{\text{nl}}^{(\text{loc})} + \text{const.} \quad (9)$$

Thus one can characterize *all* the Griffiths singularities in the disordered phase by a *single* continuously varying exponent,  $z$ . This prediction is indeed confirmed by the numerical investigations [11, 12] as demonstrated in fig. 1.



**Fig. 1. Left:** The probability distribution of the local non-linear susceptibility at a point in the disordered phase (the critical point is at  $T_c^{\text{cl}} = 3.30$ ). The parameter  $T^{\text{cl}}$  is related to the transverse field strength via the Suzuki-Trotter mapping (see [9] for details). The straight line has slope  $-0.87$  which gives via (9)  $z = 0.76$ . Since the slope is greater than  $-1$ , or equivalently  $z > 2/3$ , the average non-linear susceptibility does *diverge* at this point. **Right:** The dynamical exponent  $z$ , obtained by fitting the distributions of  $\chi^{(\text{loc})}$  and  $\chi_{\text{nl}}^{(\text{loc})}$  to Eqs. (8) and (9), is plotted for different values of  $T^{\text{cl}}$ . The estimates obtained from data for  $\chi^{(\text{loc})}$  are shown by the triangles and the estimates from the data for  $\chi_{\text{nl}}^{(\text{loc})}$  are shown by the hexagons. The two are in good agreement. The dotted vertical line indicates the critical point, obtained in Ref. [8] and the solid square indicates the estimate of  $z$  at the critical point. The dashed line is  $z = 2/3$ ; the average non-linear susceptibility diverges for  $z$  larger than this, i.e.  $T^{\text{cl}} > T_{\chi_{\text{nl}}}^{\text{cl}} \simeq 3.56$ . The solid curve is just a guide to the eye.

We see that the *average* susceptibility in the disordered phase ( $\Gamma > \Gamma_c$ ) will diverge when  $z > d$ , and the nonlinear susceptibility when  $z > d/3$ . From fig. 1 (taken from [11]) we see that in two dimensions this is indeed the case for the non-linear susceptibility in a range  $\Gamma \in [\Gamma_c, \Gamma_{\chi_{\text{nl}}}]$ . However, the numerical value of  $\Gamma_c$  and  $\Gamma_{\chi_{\text{nl}}}$  might be non-universal and so we cannot make a precise prediction for what the range of field-values, in which  $\chi_{\text{nl}}$  diverges, might be in an experiment.

In three dimensions [12] the situation is similar, although here the range of transverse field values where the nonlinear susceptibility diverges is much



smaller than in 2d. This is plausible since for increasing dimension the spectacular effects of the Griffiths singularities, which have their origin in spatially isolated clusters, becomes weaker and seem to vanish in the mean field theory.

Finally we would like to emphasize that due to the divergent behavior of the linear or higher susceptibilities in part of the quantum Griffiths phase we expect this effect to be observable also in an experiment with a macroscopic but finite system. It has been argued by Imry [24] that the Griffiths singularity occurring in a *classical* diluted Ising magnet is an artifact of the thermodynamic limit procedure. What is meant here is the essential singularity in a *static* quantity (like the magnetization or susceptibility). In essence the argument is that in order for these effects to be observable one needs a macroscopic cluster, which would occur only once in an astronomically large collections of finite samples. However, since in the *quantum* case, which we consider here, the statics is inextricably mixed with the *dynamics*, static quantities are much more sensible with respect to the existence of strongly coupled regions even of modest size. The distribution of cluster sizes  $n$  is still effectively cut off around  $n_{\max} \sim \log N$ , where  $N = L^d$  is the system size. However, such a *typical* cluster, which occurs with probability  $\mathcal{O}(1)$  leads to a (local) nonlinear susceptibility of  $\chi_{nl}^{(\text{loc})} \sim N^{3\sigma'}/\zeta$ . For a macroscopic sample ( $N \sim 10^{23}$ ) this is a huge number, which should render the divergence predicted for an infinite sample observable also in a macroscopic *typical* system (in contrast to the mere non-analyticities in the classical case).

## 4 Conclusions

The quantum phase transition occurring at zero temperature in transverse field Ising spin glasses can be described by a set three independent exponents that have been determined numerically. The dynamical exponent  $z$ , connecting time- or energy scales with a spatial diverging length is finite in  $d > 1$  and infinite in the one-dimensional model. The critical point is surrounded by a quantum Griffiths phase, where various susceptibilities diverge. These divergences can be characterized by a single continuously varying exponent  $z$ . Its limiting value seems to be identical to the critical value, which is analytically established in 1d. The most important observation is that, although a Griffiths phase should be present in all random magnets, this is the first numerical verification of some of its theoretically predicted features. We would not be surprised if the divergences we found in the quantum Griffiths phase could also be measured in an appropriate experiment. It is interesting to speculate on whether the possible divergence of the non-linear susceptibility in part of the disordered phase might be related to the difference between the experiments [13] which apparently do not find a strong divergence of  $\chi_{nl}$  at the critical point, and the simulations [8], [9] which do. Certainly more work in this direction has to be done.

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