QUANTUM SPIN GLASSES IN FINITE DIMENSIONS

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ABSTRACT

The Ising spin glass model in a transverse field has a zero temperature phase transition driven solely by quantum fluctuations. This quantum phase transition occuring at a critical transverse field strength has attracted much attention recently. We report the progress that has been made via Monte Carlo simulations of the finite dimensional, short range model.

The most frequently discussed spin glass models are classical systems for which quantum fluctuations can be neglected[1]. In most cases this is correct, namely as long as $T_c > 0$. The reason for that is that critical fluctuations at the transition occur at a frequency ω_c ($= \tau^{-1}$, where τ is the relaxation time) with $\hbar\omega_c \ll k_B T$ since $\omega_c \to 0$ as $T \to T_c$ due to critical slowing down. Hence any finite temperature will destroy quantum coherence and the system will behave classically. Very recently however, spin glasses began to enter the quantum regime[2].

The interesting theoretical question is: What are the effects of quantum mechanics on the physics of strongly disordered systems at zero temperature, where no heat bath is present and hopping over energy barriers is replaced by tunneling through them quantum-mechanically? The renewed interest in spin glasses in the quantum regime was kindled by a series of recent experiments[3] on the dipolar Ising magnet $\mathrm{Li}_x\mathrm{Ho}_{1-x}\mathrm{YF}_4$, where T_c was driven down to zero by the application of a transverse magnetic field Γ (see the phase diagram depicted in figure 1). Therefore it became possible to study the *zero* temperature phase transition occuring for critical transverse field strength Γ_c by simply tuning the external field. This quantum phase transition lies within a different universality from the usually studied (classical) spin glass transition at finite temperatures and it turns out that their properties differ significantly.

The above mentioned experiments can be described by the model Hamiltonian of an Ising spin glass in a transverse field[3]

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x - h\sum_i \sigma_i^z \;, \tag{1}$$

where the σ_i are Pauli spin matrices, Γ is the strength of the transverse field and h is

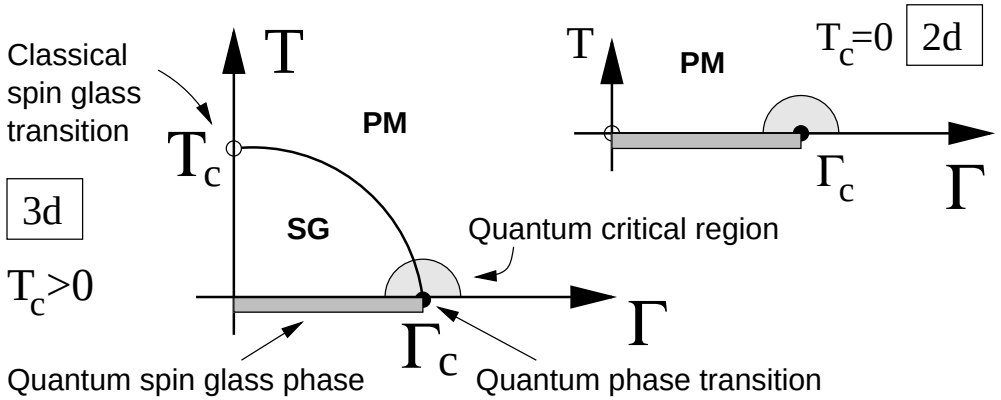

Fig. 1. Typical phase digram of a three– (left) and two– (right) dimensional quantum Ising spin glass in a transverse field.

a longitudinal magnetic field used to define magnetic susceptibilities but usually set to zero. Obviously, for $\Gamma = 0$ the quantum-mechanical Hamiltonian (1) is diagonal in the z-representaion of the spin operators, which in this case can simply be replaced by their eigenvalues ± 1 (after rescaling the couplings) giving exactly the classical EA-model in d dimensions: $H = -\sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z$, where now $S_i = \pm 1$ are Ising spin variables. In this way the transverse field introduces quantum mechanics into the spin glass problem and the value of Γ tunes the strength of the quantum fluctuations. At zero temperature and $\Gamma = 0$ the system described by (1) will be in its uniquely determined ground state, which is identical to the classical ground state of the EA-spin glass model. In this case one has $\langle \sigma_i^z \rangle = \pm 1$ for all sites i and therefore $q_{EA} = [\langle \sigma_i^z \rangle^2]_{\rm av} = 1$, where $\langle \cdots \rangle$ means the quantum-mechanical expectation value.

If we switch on the transverse field ($\Gamma > 0$) the Hamiltonian (1) is not diagonal in the z-representation any more and its ground state will be a superposition of the classical ground state plus various excited states, which describes the quantum-mechanical tunneling at zero temperature between the local energy minima of the classical Hamiltonian. Furthermore $|\langle \sigma_i^z \rangle| < 1$ since the transverse field tries to align the spins in the x-direction and therefore $q_{EA} = [\langle \sigma_i^z \rangle^2]_{\rm av} < 1$. Increasing Γ diminishes the EA-order parameter q_{EA} and for some critical value Γ_c it will be zero: $q_{EA} = 0$ for $\Gamma \geq \Gamma_c$. This is the zero temperature phase transition we are interested in and obviously we cannot expect that its critical properties have anything in common with the finite temperature classical spin glass transition.

In order to describe this zero-temperature transition one introduces a quantity measuring the distance from the critical transverse field strength (at $T = 0$) $\delta = (\Gamma - \Gamma_c)/\Gamma_c$. If one assumes a conventional second order phase transition one has $q_{EA} \sim |\delta|^\beta$ and spatial correlations decay on a characteristic length scale that diverges at the critical point as usual: $\xi \sim |\delta|^{-\nu}$ and these exponents defined so far would be

sufficient to describe the static critical behavior of a classical spin glass transition (provided hyperscaling holds). However, at a zero temperature transition driven solely by quantum fluctuations static and dynamic quantities are linked in such way that the introduction of a characteristic time-scale (or inverse frequency) is necessary: $\xi_\tau \sim \xi^z \sim |\delta|^{-z\nu}$, where z is the dynamical exponent. This will become more evident below, when we consider an equivalent classical model.

Much work in the past has been devoted to the infinite range model[4] and the phase-diagram in the Γ-T-plane looks similar to the one shown in figure 1, i.e. for low enough temperature T and field Γ one finds a transition line separating a paramagnetic phase from a spin glass phase. Recent work[5] focused on the zero-temperature critical behavior and calculated the critical exponents $\gamma = 1/2$ (with multiplicative logarithmic corrections), $\beta = 1$ and $z\nu = 1/2$.

In two and three dimensions, which are most relevant for the above mentioned experiments, no analytical results are known. For this reason extensive Monte Carlo simulations have been performed recently in two dimensions by Rieger and Young[6] and in three dimensions by Guo, Bhatt and Huse[7]. Usually the investigation of quantum systems via Monte Carlo methods are hampered by various deficiencies, the sign problem being the most notorious one in this respect (see[8] for a review). In studying the Ising spin glass in a transverse field however, one can exploit the fact that it can be mapped exactly onto a classical Ising model described by a *real* Hamiltonian. Using the Suzuki-Trotter formula[9] one can easily show that the ground state energy of the d–dimensional quantum mechanical model (1) is equal to the free energy of a $(d+1)$–dimensional classical model, where the extra dimension corresponds to imaginary time, i.e.

$$-\frac{E(T=0)}{L^d} = \lim_{T\to 0} \frac{T}{L^d} \mathrm{Tr}\; e^{-\beta H} = \frac{1}{\Delta\tau}\frac{1}{L_\tau L^d} \mathrm{Tr}\; e^{-\mathcal{S}} \tag{2}$$

where the imaginary time direction has been divided into L_τ time slices of width $\Delta\tau$ ($\Delta\tau L_\tau = \beta$), and the effective classical action, $\mathcal{S}$, is given by

$$\mathcal{S} = -\sum_\tau \sum_{\langle ij\rangle} K_{ij} S_i(\tau) S_j(\tau) - \sum_\tau \sum_i K S_i(\tau) S_i(\tau+1) - \sum_\tau \sum_i H S_i(\tau)\;, \tag{3}$$

where the $S_i(\tau) = \pm 1$ are classical Ising spins, the indices i and j run over the sites of the original d–dimensional lattice and $\tau = 1, 2, \ldots, L_\tau$ denotes a time slice. Moreover it is $K_{ij} = \Delta\tau J_{ij}$, $H = \Delta\tau h$ and $\exp(-2K) = \tanh(\Delta\tau\Gamma)$. One has the *same* random interactions in each time slice. In order to fulfill the second equality in (2) precisely, one has to perform the limit $\Delta\tau \to 0$, which implies $K_{ij} \to 0$ and $K \to \infty$. However, the universal properties of the phase transition are expected to be independent of $\Delta\tau$ so we take $\Delta\tau = 1$ and set the standard deviation of the K_{ij} to equal K. Thus K, which physically sets the relative strength of the transverse field and exchange terms in (1), is like an inverse "temperature" for the effective classical model in (3).

One sees that the (d+1)-dimensional classical model (3) should order at low "temperature" (or coupling constant K) like a spin glass in the d spatial dimensions and ferromagnetically in the imaginary time direction. From this one concludes the existence of two different diverging length-scales in the classical model (3): one for the spatial (spin glass)-correlations, which is ξ, and one for imaginary time (ferromagnetic) correlations, which is ξ_τ. Thus in the representation (3) the link between statics and dynamics in the original quantum model (1) becomes most obvious. Correspondingly, to analyze the critical properties of the extremely anisotropic classical model (3) one has to take into account these two length scales via anisotropic finite size scaling[10].

Monte Carlo simulations of the classical model (3) are straightforward but it turns out that sample-to-sample fluctuations are significant, so one has to do an extensive disorder average[6,7]. However, the finite size scaling analysis is complicated by the existence of two diverging length scales ξ and ξ_τ and one has to deal with two independent scaling variables: as usual L/ξ and in addition the shape (or aspect ratio) L_τ/L^z of the system[10]. Thus, with the usual definition of a spin glass overlap $Q = L^{-d}L_\tau^{-1}\sum_{i,\tau} S_i^a(\tau)S_i^b(\tau)$ (a and b are two replicas of the same system) for the classical system, the dimensionless combination of moments of the order-parameter $g_{\rm av}$ obeys

$$g_{\rm av}(K, L, L_\tau) = 0.5[3 - \langle Q^4\rangle/\langle Q^2\rangle^2]_{\rm av} \sim \tilde{g}_{\rm av}(\delta L^{1/\nu}, L_\tau/L^z) \; . \tag{4}$$

Here $\langle\cdots\rangle$ means the thermal average and $[\cdots]_{\rm av}$ means the disorder average. In isotropic systems one has $z = 1$, which makes the aspect ratio constant to one for the choice $L = L_\tau$ and in order to determine the critical coupling K_c one exploits the fact that $g_{\rm av}(K, L, L)$ becomes independent of L for $K = K_c$. In the present case of a very anisotropic system z is not known a priori and one has to vary three different system parameters to obtain an estimate for K_c and z (and other exponents). The following method[6,7] enhances the efficiency of such a search in a three-parameter space and also produces reliable estimates for the quantities of interest: In the limit $L_\tau \gg L^z$ the classical $(d + 1)$-dimensional classical system is quasi-one-dimensional, and in the limit $L_\tau \ll L^z$ the system is quasi-d-dimensional and well above its transition "temperature" in d dimensions (which is even zero for $d = 2$). Therfore one has $\tilde{g}_{\rm av}(x, y) \to 0$ both for $y \to 0$ and for $y \to \infty$. Hence, for fixed x, $\tilde{g}_{\rm av}(x, y)$ must have a maximum for some value $y = y_{\rm max}(x)$. The value of this maximum decreases with increasing L in the disordered phase $K < K_c$ (where $\delta = (K_c/K - 1) > 0$) and increases with increasing L in the ordered phase. This criterion can be used to estimate the critical coupling, as exemplified in figure (2). If one plots $g_{\rm av}(K_c, L, L_\tau)$ versus L_τ/L^z with the correct choice for the dynamical exponent z, one obtains a data-collaps for all system sizes L. Finally one uses systems with fixed aspect ratio L_τ/L^z to determine critical exponents via the usual one–parameter finite size scaling.

Various scaling predictions can be made if one supposes a conventional second

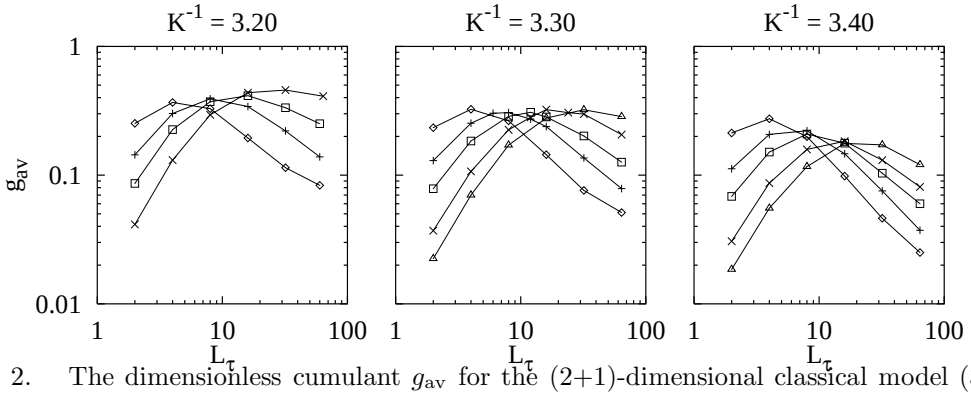

Fig. 2. The dimensionless cumulant $g_{\rm av}$ for the (2+1)-dimensional classical model (3) for three different values of the coupling constant versus the system size L_τ in the imaginary time direction. The system size in the space direction is $L = 4$ ($\diamond$), 6 (+), 8 ($\Box$), 12 ($\times$) and 16 ($\triangle$). Since the maximum of $g_{\rm av}(L_\tau)$ is roughly independent of L at $K^{-1} \approx 3.30$ one concludes that the latter value is the critical coupling constant.

order phase transition to occur at some critical "temperature" K_c for the classical model. Let us assume that we are *at* the critical point $K = K_c$ and the aspect ratio stays constant $L_\tau \propto L^z$. Then the order parameter scales with system size as $q_{EA} = [|\langle Q\rangle|]_{\rm av} \sim L^{-\beta/\nu}$ and the corresponding susceptibility $\chi_{SG} = L_\tau L^d[\langle Q\rangle^2]_{\rm av} \sim L^{\gamma/\nu}$ with $\gamma/\nu = d + z - 2\beta/\nu$. The equal time correlation function in the infinite system decays like $C(r) = [\langle S_i(\tau)S_{i+r}(\tau)\rangle^2]_{\rm av} \sim r^{-(d+z-2+\eta)}$, from which one obtains by integrating over r the scaling relation $2\beta/\nu = d + z - 2 + \eta$. The (imaginary)-time-dependent autocorrelation function of the infinite system decays like $G(t) = [\langle S_i(\tau)S_i(t+\tau)\rangle]_{\rm av} \sim t^{-(d+z-2+\eta)/2z}$ and by integrating over t one gets the uniform susceptibility $\chi_F(\omega = 0) = \partial[\langle\sigma_i^z\rangle]_{\rm av}/\partial h \sim L^{-\gamma_f/\nu}$ with $\gamma_f = z - \beta/\nu$. Thus χ_f will diverge if $z > \beta/\nu$.

The nonlinear susceptibility $\chi_{nl} = \partial^3[\langle\sigma_i^z\rangle]_{\rm av}/\partial h^3 \sim L^{-\gamma_{nl}/\nu}$ is most relevant for the experiments[3]. This quantity, also given by $\chi_{nl} = [3\langle M^2\rangle^2 - \langle M^4\rangle]_{\rm av}/L^d$, with $M = \sum_{i,\tau} S_i(\tau)$, can be shown[6] to scale in the same way as $L^d L_\tau^3[\langle Q^2\rangle]_{av}$, which yields the scaling relation $\gamma_{nl} = \nu(2 - \eta + 2z)$. The nonlinear susceptibility of the infinite system obeys $\chi_{nl}(T,\delta) \sim \delta^{-\gamma_{nl}}\tilde{\chi}_{nl}\left(T/\delta^{z\nu}\right)$ with $\tilde{\chi}_{nl}(x) \to const.$ for $x \to 0$ and $\tilde{\chi}_{nl}(x) \to x^{-\gamma_{nl}/z\nu}$ for $x \to \infty$. By setting $\Gamma = \Gamma_c$ one gets $\chi_{nl} \sim T^{-\gamma_{nl}/z\nu}$ and similarily $\chi_F \sim T^{-\gamma_f/z\nu}$.

In table 1 we list the results obtained so far in various dimensions. The symbol *div.* in the second column means that first and higher derivatives of the magnetization diverge already in the disordered phase. The word *finite* means that in three dimensions and for d larger than the upper critical dimension the uniform susceptibility does not diverge at the critical point. The results in the second column[12] were obtained within a renormalization group calculation, those in columns 3 to 5 with Monte Carlo simulations[13,6,7], column 6 shows the result of a Migdal-Kadanoff RNG

calculation and the last column depicts analytical results from mean-field theory[5]. Note that in the case $d = 1$ we refer to the non-frustrated random transverse Ising chain, where the order parameter is the magentization instead of the spin glass overlap and the exponents listed refer to the critical behavior of quantities that are defined accordingly.

Table 1. Summary of critical exponents characterizing the quantum phase transition of the transverse field Ising spin glass in finite dimensions

	d=1 RG[12]	d=1 MC[13]	d=2 MC[6]	d=3 MC[7]	d=3 MK[11]	d≥8 MFT[5]
z	∞	~ 1.7	1.50 ± 0.05	~ 1.3	~ 1.4	2
ν	2	~ 1.0	1.0 ± 0.1	~ 0.8	~ 0.87	1/4
η	$0.38\ldots$	0.40 ± 0.03	0.50 ± 0.05	~ 0.9	—	2
β/ν	$0.19\ldots$	0.18 ± 0.02	1.0 ± 0.1	~ 1.6	~ 1.5	1/2
γ	*div.*	2.3 ± 0.1	~ 1.5	~ 0.9	~ 1.2	1/2
γ_f	*div.*	—	~ 0.5	*finite*	—	*finite*
γ_{nl}	*div.*	—	~ 4.5	~ 3.5	—	—

These results imply in three dimensions a strong divergence of the nonlinear susceptibility when approaching $T = 0$: $\chi_{nl} \sim T^{-2.7}$ (since $\gamma_{nl}/\nu z \approx 2.7$), with a power that is very close to the one for classical Ising spin glasses (~ 2.9, ref.[1]). This is in striking contradiction to the observation made in the experiments mentioned in the introduction[3] and in order to clarify this discrepancy further work is necessary.

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