Zero–Temperature Quantum Phase Transition of a Two–Dimensional Ising Spin–Glass

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Abstract

We study the quantum transition at $T = 0$ in the spin-$\frac{1}{2}$ Ising spin–glass in a transverse field in two dimensions. The world line path integral representation of this model corresponds to an effective classical system in (2+1) dimensions, which we study by Monte Carlo simulations. Values of the critical exponents are estimated by a finite-size scaling analysis. We find that the dynamical exponent, $z$, and the correlation length exponent, $\nu$, are given by $z = 1.5 \pm 0.05$ and $\nu = 1.0 \pm 0.1$. Both the linear and non-linear susceptibility are found to diverge at the critical point.

75.50.Lk, 75.10.Nr, 05.30.–d, 75.40.Gb
Much attention has been given to the finite temperature transition in spin glass systems, see e.g. [1], and reasonable agreement between theory and experiment has been obtained. This transition is driven by thermal fluctuations controlled by the temperature. However, one can also control the strength of quantum fluctuations by altering parameters in the system. Turning up the quantum fluctuations will decrease the transition temperature $T_c$, eventually forcing it to zero. Critical fluctuations near the transition are classical as long as $T_c > 0$, because they occur at a frequency $\omega$ satisfying $\hbar \omega \ll k_B T$ [2]. Consequently, the universality class is that of the classical problem except if one tunes through the transition at $T = 0$. This quantum universality class has not been much studied for the spin glass problem, though other quantum phase transitions, such as the metal–insulator [3] and bose–glass [4] transitions, have attracted a lot of attention. Most theoretical work on the quantum spin glass [5,6] has been confined to the infinite range model, which is expected to describe the transition in a short range system of sufficiently high space dimension.

Recently, however, the quantum spin glass transition was studied experimentally [7] in an Ising system with dipolar couplings in which $T_c$ was driven to zero by applying an effective transverse field. Interestingly, the non-linear susceptibility, $\chi_{nl}$, which diverges at the finite-$T$ classical transition [4], was found not to diverge, or at least to diverge much less strongly than in the classical case. Furthermore, the phase transition in a quantum Ising spin system in (1+1) dimensions has recently been studied in detail [8], see also [9]. It is found that both the linear and non-linear susceptibility diverge not only at the critical point but also in part of the disordered phase. Although this model does not have frustration, and therefore might miss some of the spin glass physics, it is interesting to investigate whether similar behavior also occurs higher dimensions. It is therefore an appropriate time to study the quantum Ising spin glass and here we report on results of Monte Carlo simulations on a short range model in (2+1) dimensions. Similar calculations and analysis have also been performed in (3+1) dimensions [10].

The model system studied in this paper, which is appropriate for the experimental system, LiHo$_x$Y$_{1-x}$F$_4$ [7], is the Ising spin glass in a transverse field with Hamiltonian
\[
H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x ,
\]
(1)

where the \( \sigma_i \) are Pauli spin matrices, \( \Gamma \) is the strength of the transverse field and the nearest neighbor interactions, \( J_{ij} \), are independent random variables with a Gaussian distribution of mean zero and standard deviation unity.

If \( \Gamma = 0 \) the Hamiltonian in (1) is the classical two dimensional Ising spin–glass. The ground state is doubly degenerate (the two states being related by global spin–flip symmetry) so, at \( T = 0 \), the Edwards–Anderson order parameter [1] \( q_{EA} = [\langle \sigma_i^z \rangle^2]_{av} \) is unity. We denote a statistical mechanics average by angular brackets, \( \langle \cdots \rangle \), and an average over the quenched disorder by square brackets, \( [\cdots]_{av} \). Switching on the transverse field mixes the eigenstates of \( \sigma^x \) and thus diminishes the EA–order parameter, causing it to vanish at some finite value, \( \Gamma_c \). This is the transition that we study here. Details of the calculations will be given elsewhere [12].

It is well known [13] 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.

\[
- \frac{E(T = 0)}{L^d} = \lim_{T \to 0} \frac{T}{L^d} \text{Tr} \ e^{-\beta H} = \frac{1}{\Delta \tau} \frac{1}{L_{\tau} L^d} \text{Tr} \ e^{-S}
\]
(2)

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

\[
S = - \sum_{\tau} \sum_{\langle ij \rangle} K_{ij} S_i(\tau) S_j(\tau) - \sum_{\tau} \sum_i K S_i(\tau) S_i(\tau + 1) ,
\]
(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. In Eq. (3), \( K_{ij} = \Delta \tau J_{ij} \) and \( \exp(-2K) = \tanh(\Delta \tau \Gamma) \). Note that we have the same random interactions in each time slice. We should take the limit \( \Delta \tau \to 0 \), which implies \( K_{ij} \to 0 \) and \( K \to \infty \). This extremely anisotropic limit is inconvenient for calculations but universal properties 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).

We study the model (3) in $d = 2$ dimensions by Monte–Carlo simulations on a simple cubic lattice of size $L \times L \times L_\tau$ using periodic boundary conditions. Since various quantities of interest show a very strong dependence on the disorder realization we have to average over a large number of samples — we took 2560 samples for each temperature and size. The largest systems were $20 \times 20 \times 50$, where we used up to $10^5$ Monte Carlo sweeps for equilibration plus $10^5$ sweeps for measurements, which were performed every 20 sweeps. Equilibration was checked with standard methods [11]. The simulations were performed on a large transputer array (GCell1024 from Parsytec).

Because the system in (3) is very anisotropic, it is expected to have two different diverging scales: one is the correlation length in the space direction, $\xi \sim \delta^{-\nu}$, where $\delta = K_c / K - 1$ is the distance from the critical point $K_c$, and the other is the correlation time, $\xi_\tau$, in the (imaginary) time direction, where $\xi_\tau \sim \xi^z$ with $z$ the dynamical exponent. According to a finite size scaling hypothesis extended to anisotropic systems [14], various 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 $L_\tau / L^z$. 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, and we follow an efficient method of doing this suggested by Huse [15].

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

$$Q = \frac{1}{L^d L_\tau} \sum_{i,\tau} S_i^{(1)}(\tau) S_i^{(2)}(\tau) , \quad (4)$$

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

$$g = 0.5 \left[ 3 - \langle Q^4 \rangle / (\langle Q^2 \rangle)^2 \right] . \quad (5)$$
The disorder averaged quantity, $g_{av} = [g]_{av}$ [13], obeys the finite size scaling form

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

and has the property [14] that it vanishes in the disordered phase for $L \to \infty$, and tends to a finite value in the ordered phase. Consequently, $\bar{g}(x, y)$ 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 $\tau$ direction, which is also disordered). Hence, $\bar{g}(x, y)$ must have a maximum at some value of $y$ for fixed $x$. 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. We use this criterion to estimate the critical coupling which we find is given by $K_c^{-1} = 3.275 \pm 0.025$. The data are shown in Fig. 1. Furthermore, at the critical point, the values of $L$ and $L_\tau$ for which $\bar{g}$ is a maximum are related by $L_\tau \sim L^z$. By this method we determine the dynamical exponent and get $z = 1.50 \pm 0.05$. The finite-size scaling hypothesis (6) can be checked a posteriori by a scaling plot for $g_{av}$ at $K_c$ as shown in Fig. 2.

Systems with fixed aspect ratio, $L_\tau/L^z$, can be used them to determine critical exponents via the usual one-parameter finite-size scaling. First of all, from Eq. (8) the derivative of $\bar{g}$ with respect to $K$ at $K_c$ gives $\nu$ and we find $\nu = 1.0 \pm 0.1$, see Fig. 3. The rigorous inequality $\nu \geq 2/d$ [17] is therefore satisfied, perhaps as an equality.

There are various susceptibilities that one can define for this problem, with different numbers of integrations over imaginary time. For example, the second moment of $Q$, $\chi_Q = L^d L_\tau[\langle Q^2 \rangle]_{av}$, has a single integral over $\tau$. Defining the exponent $\gamma_Q$ by $\chi_Q \sim \delta^{-\gamma_Q}$, then, at the critical point, the size dependence is given by $\chi_Q \sim L^{2-\eta}$ where $\gamma_Q = (2-\eta)\nu$. On the other hand, the equal time spin glass correlation function, $C_0 = \sum_{i1}[\langle S_{i0}(\tau_0)S_i(\tau_0) \rangle^2]_{av}$, has no $\tau$ sum and so varies as $L^{2-\eta-z}$ [18]. Consider next the overlap

$$q^{ab} = \frac{1}{L^d L_\tau^2} \sum_{i,\tau,\tau_2} S_i^{(a)}(\tau_1)S_i^{(b)}(\tau_2).$$

(7)
which involves a double sum over $\tau$. The corresponding susceptibility, $\chi_q = L^d L^2 \langle (q^{12})^2 \rangle_{av}$, involves two time integrals so it should vary as $L^{2-\eta+z}$ at criticality [18]. The experimentally measured non-linear susceptibility is the fourth derivative of the free energy with respect to a field coupling to $S_z^z$, and so is related to the fourth order cumulant of the total magnetization by standard linear response theory, $\chi_{nl} = \frac{\langle M^4 \rangle - 3 \langle M^2 \rangle^2}{(L^d L^2 \tau)}$, where $M = \sum_{i,\tau} S_i(\tau)$. Since the disorder average gives zero unless each spin occurs an even number of times, $\chi_{nl}$ can be expressed (neglecting a local piece which diverges less strongly) as

$$\chi_{nl} = L^d L^2 \left[ \langle (q^{12})^2 \rangle - \frac{1}{4} \langle (q^{11} - q^{22})^2 \rangle \right]_{av} \tag{8}$$

which has three sums over $\tau$ and so should diverge at criticality like $L^{2-\eta+2z}$ [18]. Fig. 4 shows data and fits for $C_0, \chi_q, \chi_Q$ and $\chi_{nl}$ at criticality. All the data are consistent with the exponent values, $\eta \simeq 0.5, z \simeq 1.5$. In particular, $\chi_{nl} \sim L^4.7$ at criticality, or equivalently $\chi_{nl} \sim L^{3.1}$ using $z = 1.5$. Since $L_r \propto \beta$, $\chi_{nl}$ varies as $T^{-3.1}$ for $T \to 0$ at the critical transverse field $\Gamma_c$, which is quite a strong divergence. Note that, by contrast, the equal time correlation function does not diverge (or only does so marginally). This is because spatial correlations fall off quite rapidly at criticality, like $r^{-2}$, as we have verified directly.

According to scaling theory [4], the (unsquared) on-site correlation function at the critical point, $C(\tau) = \langle S_i(0) S_i(\tau) \rangle_{av}$ varies as $\tau^{-(d+z-2+\eta)/(2z)}$, or $\tau^{-2/3}$ using our values for the exponents. Integrating this over $\tau$ to get the uniform susceptibility, $\chi_F [19]$, $\chi_F = \sum_{\tau} C(\tau)$, one finds a divergence of the form $L_r^{1/3}$, or $\chi_F \sim T^{-1/3}$ as $T \to 0$ at $\Gamma = \Gamma_c$. Thus, in contrast to the classical spin glass [1], the uniform susceptibility diverges at the quantum spin glass transition in (2+1) dimensions.

Similar calculations and analysis have been performed on a (3+1) dimensional model [10], with results which are quite similar to ours, though the numerical values for exponents are somewhat different as expected. The main qualitative difference is that the uniform susceptibility does not diverge in (3+1) dimensions. Both our work and the results in (3+1) dimensions [10] show a substantial divergence of $\chi_{nl}$, which appears to be rather different
from experiment [7]. The reason for this discrepancy is unclear at present. For future work it will be interesting to investigate whether the uniform and spin glass susceptibilities diverge in part of the disordered phase, as happens in $d = (1+1)$ because of Griffiths singularities arising from rare regions which are more strongly coupled than the average [8].

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We would like to thank David Huse for very enlightening discussions on this point.

We also tried averaging the numerator and denominator in Eq. (5) separately over the disorder, as was done in the classical spin glass [11]. An analysis gives similar results [12] but with worse statistics because of strong sample–to–sample fluctuations.

The divergence of the various susceptibilities can also be obtained by noting that $Q$ (and $q$ defined in Eq. (7)) is the order parameter for this problem and so, according to finite-size scaling, both $\langle Q^2 \rangle_{\text{av}}$ and $\langle q^2 \rangle_{\text{av}}$ vary as $L^{-2\beta/\nu}$ at criticality. Note also that the equal time correlation function $C_0$ is of the form $L^d$ times the square of the order parameter. In addition, $L_\tau \propto L^z$, and, according to hyperscaling with $d$ replaced by $d + z$ [4], one has $2\beta/\nu = d + z - 2 + \eta$. These considerations then lead to the exponents summarized in the caption to Fig. 4.

Contributions to $\chi_F$ of the type $\langle [S_i(0)S_j(\tau)] \rangle_{\text{av}}$, where $i \neq j$, vanish for a symmetric bond distribution so the uniform susceptibility is equal to the local (on–site) susceptibility.

N. Read (private communication).
FIGURES

FIG. 1. The averaged cumulant $g_{av}(K, L, L_{\tau})$ for three different coupling constants ($K^{-1}=3.20$ left, $K^{-1}=3.30$ middle and $K^{-1}=3.40$ right) and various systems sizes ($L=4$ (⋄), $L=6$ (+), $L=8$ (□), $L=12$ (∗) and $L=16$ (△)) as a function of $L_{\tau}$. The maximum increases with $L$ for $K^{-1}=3.20$, which implies $K_{c}^{-1}>3.20$, and it decreases with increasing $L$ for $K^{-1}=3.40$, so $K_{c}^{-1}<3.40$. We have also data for $K^{-1}=3.25$, from which we conclude that $K_{c}^{-1}$ is between 3.25 and 3.30. The errorbars are smaller than the symbols.

FIG. 2. A scaling plot of $g_{av}(K, L, L_{\tau})$ at $K^{-1}=3.30 \simeq K_{c}^{-1}$ as a function of the scaled system size in the (imaginary) time direction $L_{\tau}/L_{\tau}^{max}$. For each lattice size, $L_{\tau}^{max}$ is chosen so that all the data collapses on to a single curve. The sizes are ($L=4$ (⋄), $L=6$ (+), $L=8$ (□), $L=12$ (∗) and $L=16$ (△)). The inset shows the dependence of $L_{\tau}^{max}$ as a function of $L$. From Eq. (6) the slope is equal to the dynamical exponent $z$ and a fit gives $z=1.50 \pm 0.05$.

FIG. 3. The derivative of $g_{av}$ with respect to $K^{-1}$ at $K^{-1}=3.30 \simeq K_{c}^{-1}$, for systems of size $4 \times 4 \times 4, 6 \times 6 \times 8, 8 \times 8 \times 14, 12 \times 12 \times 24$ and $16 \times 16 \times 34$, which have a roughly constant aspect ratio, $L_{\tau}/L^{2}$, since $z \simeq 1.5$. A least squares fit of the data to a straight line yields a slope of $1/\nu = 1.0 \pm 0.1$.

FIG. 4. The equal time correlation function, $C_{0}$, and the susceptibilities $\chi_Q, \chi_q$ and $\chi_{nl}$ as a function of $L$ close to the critical point, $K^{-1}=3.30 \simeq K_{c}^{-1}$, on a double logarithmic plot. The slopes are expected to be $2-\eta - z$, $2-\eta$, $2-\eta + z$, and $2-\eta + 2z$, respectively. A least squares fit gives the values $0.2 \pm 0.1, 1.4 \pm 0.1, 3.1 \pm 0.1$ and $4.7 \pm 0.2$, which are consistent with the exponents, $\eta \simeq 0.5, z \simeq 1.5$. The system sizes are the same as in Fig. 3.
Fig. 2
Fig. 3
Fig. 4