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

H. Rieger
Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany

A. P. Young
Department of Physics, University of California, Santa Cruz, California 95064
(Received 5 April 1994)

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, ν, are given by $z=1.5\pm0.05$ and $\nu=1.0\pm0.1$. Both the linear and nonlinear susceptibility are found to diverge at the critical point.

PACS numbers: 75.50.Lk, 05.30.−d, 75.10.Nr, 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 ω satisfying $\hbar\omega\ll k_BT$ [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 nonlinear susceptibility, $\chi_{\rm nl}$, which diverges at the finite-T classical transition [1], 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 nonlinear 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 in 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, $LiHo_xY_{1-x}F_4$ [7], is the Ising spin glass in a transverse field with Hamiltonian

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

where the σ_i are Pauli spin matrices, Γ is the strength of the transverse field and the nearest neighbor interactions, and 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 (EA) order parameter [1] $q_{\rm EA}=[\langle\sigma_i^z\rangle^2]_{\rm av}$ is unity. We denote a statistical mechanics average by angular brackets, $\langle\cdots\rangle$, and an average over the quenched disorder by square brackets, $[\cdots]_{\rm av}$. Switching on the transverse field mixes the eigenstates of σ^z and thus diminishes the EA order parameter, causing it to vanish at some finite value, Γ_c. This is the transition that we study here. Details of the calculations will be given elsewhere [11].

It is well known [12] 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.,

$$-\frac{E(T=0)}{L^d}=\lim_{T\to0}\frac{T}{L^d}\,\mathrm{Tr}\,e^{-\beta H}=\frac{1}{\Delta\tau}\frac{1}{L_\tau L^d}\,\mathrm{Tr}\,e^{-\mathcal{S}}\,, \tag{2}$$

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

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

0031-9007/94/72(26)/4141(4)$06.00

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 [13]. The simulations were performed on a large transputer array (GCel1024 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, ξ_τ, 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_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, and we follow an efficiency 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

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

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

$$g = 0.5[3 - \langle Q^4 \rangle / \langle Q^2 \rangle^2] . \tag{5}$$

The disorder averaged quantity, $g_{\rm av} = [g]_{\rm av}$ [16], obeys the finite-size scaling form

$$g_{\rm av}(K,L,L_\tau) = \tilde{g}_{\rm av}(\delta L^{1/\nu}, L_\tau/L^z) , \tag{6}$$

and has the property [13] 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. 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_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 $z = 1.50 \pm 0.05$. The finite-size scaling hypothesis (6) can be checked *a posteriori* by a scaling plot for $g_{\rm av}$ at K_c as shown in Fig. 2.

Systems with fixed aspect ratio, L_τ/L^z, can be used then to determine critical exponents via the usual one-

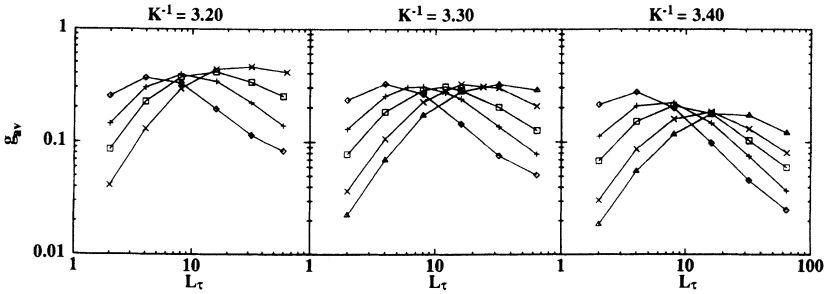

FIG. 1. The averaged cumulant $g_{\rm av}(k,L,L_\tau)$ for three different coupling constants [$K^{-1} = 3.20$ (left), $K^{-1} = 3.30$ (middle), and $K^{-1} = 3.40$ (right)] and various system sizes [$L = 4$ ($\diamond$), $L = 6$ (+), $L = 8$ ($\square$), $L = 12$ ($\times$), and $L = 16$ ($\triangle$)] as a function of L_τ. 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 also have data for $K^{-1} = 3.25$, from which we conclude that K_c^{-1} is between 3.25 and 3.30. The error bars are smaller than the symbols.

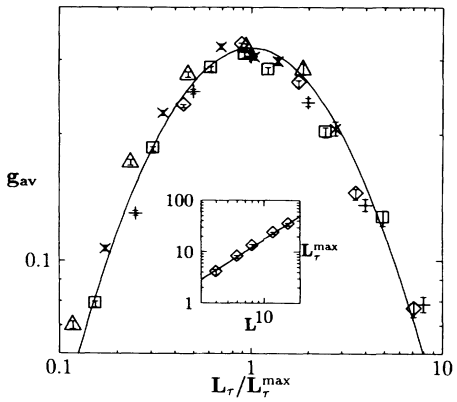

FIG. 2. A scaling plot of $g_{av}(K,L,L_\tau)$ at $K^{-1}=3.30\simeq K_c^{-1}$ as a function of the scaled system size in the (imaginary) time direction L_τ/L_τ^{max}. For each lattice size, L_τ^{max} is chosen so that all the data collapse onto a single curve. The sizes are $L=4$ ($\diamond$), $L=6$ (+), $L=8$ ($\square$), $L=12$ ($\times$), and $L=16$ ($\diamond$). The inset shows the dependence of L_τ^{max} as a function of L. From Eq. (6) the slope is equal to the dynamical exponent z and a fit gives $z=1.50\pm0.05$.

parameter finite-size scaling. First of all, from Eq. (6) the derivative of $\tilde{g}$ with respect to K at K_c gives ν and we find $\nu=1.0\pm0.1$; 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, $\chi_Q=L^dL_\tau[\langle Q^2\rangle]_{av}$, has a single integral over τ. Defining the exponent γ_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, $C_0=\sum_i[\langle S_{i_0}(\tau_0)S_i(\tau_0)\rangle^2]_{av}$, has no τ sum and so varies as $L^{2-\eta-z}$ [18]. Consider next the overlap

$$q^{ab}=\frac{1}{L^dL_\tau^2}\sum_{i,\tau_1,\tau_2}S_i^{(a)}(\tau_1)S_i^{(b)}(\tau_2)\,, \tag{7}$$

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

$$\chi_{nl}=L^dL_\tau^3[\langle(q^{12})^2\rangle-\tfrac{1}{4}\langle(q^{11}-q^{22})^2\rangle]_{av}\,, \tag{8}$$

which has *three* sums over τ and so should diverge at criticality like $L^{2-\eta+2z}$ [18]. Figure 4 shows data and fits for C_0, χ_q, χ_Q, and χ_{nl} at criticality. All the data are consistent with the exponent values, $\eta\simeq0.5$, $z\simeq1.5$. In particular, $\chi_{nl}\sim L^{4.7}$ at criticality, or equivalently $\chi_{nl}\sim L_\tau^{3.1}$ using $z=1.5$. Since $L_\tau\propto\beta$, χ_{nl} varies as $T^{-3.1}$ for $T\to0$ at the critical transverse field Γ_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.

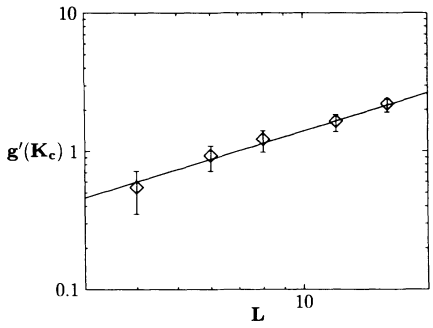

FIG. 3. The derivative of g_{av} with respect to K^{-1} at $K^{-1}=3.30\simeq K_c^{-1}$, for systems of size $4\times4\times4$, $6\times6\times8$, $8\times8\times14$, $12\times12\times24$, and $16\times16\times34$, which have a roughly constant aspect ratio, L_τ/L^z, since $z\simeq1.5$. A least squares fit of the data by a straight line yields a slope of $1/\nu=1.0\pm0.1$.

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 τ to get the uniform susceptibility, χ_F [19], $\chi_F=\sum_\tau C(\tau)$, one finds a divergence of the form $L_\tau^{1/3}$, or $\chi_F\sim T^{-1/3}$ as $T\to0$ at $\Gamma=\Gamma_c$. Thus, in contrast to the classical spin

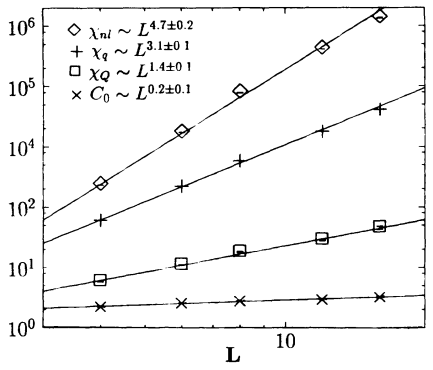

FIG. 4. The equal time correlation function C_0 and the susceptibilities χ_Q, χ_q, and χ_{nl} as a function of L close to the critical point, $K^{-1}=3.30\simeq K_c^{-1}$, on a double logarithmic plot. The slopes are expected to be $2-\eta-z$, $2-\eta$, $2-\eta+z$, and $2-\eta+2z$, respectively. A least squares fit gives the values 0.2 ± 0.1, 1.4 ± 0.1, 3.1 ± 0.1, and 4.7 ± 0.2, which are consistent with the exponents, $\eta\simeq0.5$, $z\simeq1.5$. The system sizes are the same as in Fig. 3.

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 $\chi_{\rm nl}$, 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].

We would like to thank R. Bhatt and D. Huse for many extremely valuable suggestions and discussions. We also thank N. Read for a helpful conversation. H.R. acknowledges the kind hospitality of the Physics Department of UCSC, where this work was begun, as well as the generous allocation of computing time on the transputer cluster Parsytec-GCel1024 from the center of Parallel Computer (ZPR) in Köln and the friendly user support by M. Wottawa. A.P.Y. is supported by NSF DMR-91-11576, and H.R.'s work was performed within the SFB 341 Köln-Aachen-Jülich.

[1] K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986); *Recent Progress in Random Magnets*, edited by D. H. Ryan (World Scientific, Singapore, 1992).

[2] Because of critical slowing down, the characteristic frequency tends to zero at the critical point.

[3] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[4] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).

[5] A. J. Bray and M. A. Moore, J. Phys. C **13**, L655 (1980); H. Ishii and T. Yamamoto, J. Phys. C **18**, 6225 (1985); Y. Y. Goldschmidt and P. Y. Lai, Phys. Rev. Lett. **64**, 2567 (1990).

[6] J. Miller and D. Huse, Phys. Rev. Lett. **70**, 3147 (1993); J. Ye, S. Sachdev, and N. Read, Phys. Rev. Lett. **70**, 4011 (1993).

[7] W. Wu, B. Ellmann, T. F. Rosenbaum, G. Aeppli, and D. H. Reich, Phys. Rev. Lett. **67**, 2076 (1991); W. Wu, D. Bitko, T. F. Rosenbaum, and G. Aeppli, Phys. Rev. Lett. **71**, 1919 (1993).

[8] D. S. Fisher, Phys. Rev. Lett. **69**, 534 (1993).

[9] B. M. McCoy and T. T. Wu, Phys. Rev. **176**, 631 (1968); **188**, 982 (1969); **188**, 1014 (1969); P. Hoever, W. F. Wolff, and J. Zittartz, Z. Phys. B **41**, 43 (1981); R. Shankar and G. Murthy, Phys. Rev. B **36**, 536 (1993).

[10] M. Guo, R. N. Bhatt, and D. Huse, preceding Letter, Phys. Rev. Lett. **72**, 4137 (1994).

[11] H. Rieger and A. P. Young (unpublished).

[12] M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976).

[13] R. N. Bhatt and A. P. Young, Phys. Rev. B **37**, 5606 (1988).

[14] K. Binder and J. S. Wang, J. Stat. Phys. **55**, 87 (1989).

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

[16] We also tried averaging the numerator and denominator in Eq. (5) separately over the disorder, as was done in the classical spin glass [13]. An analysis gives similar results [11] but with worse statistics because of strong sample-to-sample fluctuations.

[17] J. T. Chayes, L. Chayes, D. S. Fisher, and T. Spencer, Phys. Rev. Lett. **57**, 299 (1986).

[18] 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 $[\langle Q^2\rangle]_{\rm av}$ and $[\langle q^2\rangle]_{\rm av}$ 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.

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