PHYSICAL REVIEW LETTERS

VOLUME 64 | 21 MAY 1990 | NUMBER 21

Ising Spin Glass in a Transverse Field: Replica-Symmetry-Breaking Solution

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(Received 19 March 1990)

The replica-symmetry-breaking (RSB) solution of the infinite-range Ising spin glass in the presence of a transverse field is obtained. The quenched free energy and the phase boundary of the glass transition temperature versus the transverse field are calculated at first-step RSB without using the static approximation. We demonstrate that replica symmetry (RS) has to be broken in the spin-glass phase by comparing the free energies of the RSB and RS solutions. No evidence is found to support an intermediate spin-glass phase with replica symmetry.

PACS numbers: 05.20.Dd, 05.30.Fk, 75.40.Cx, 75.50.Lk

There has been a growing interest in the theory of quantum spin glasses in recent years.[1-9] In particular, there is much interest in the Ising spin glass with a transverse field,[3-9] which is a model for the proton glasses. An example[10] is the mixed hydrogen-bonded ferroelectric $Rb_{1-x}(NH_4)_xH_2PO_4$ system in which a spin-glass phase has been observed. The system is a random mixture of ferroelectric and antiferroelectric materials and can be modeled by the Ising spin glass in a transverse field. The tunneling effect of the proton between the two minima (the two Ising spin states) of the hydrogen bond can be represented by the transverse field.[11,12] This model is particularly suitable to understand the quantum nature of spin glasses because of the fact that at zero transverse field the model reduces to the purely classical Ising spin glass. The simplest case is the infinite-range model in which any two spin pairs are interacting. Classically (no transverse field), this is the Sherrington-Kirkpatrick (SK) model[13] which is well described by Parisi's replica-symmetry-breaking (RSB) solution.[14] The novel features like coexistence of many almost-degenerate thermodynamic states separated by huge free-energy barriers and a wide spectrum of dynamical time scales are contained in this solution. Thus it is interesting to understand whether such a phase-space picture remains true if quantum effects are included; will the quantum fluctuations be strong enough to cause tunneling between these free-energy barriers and destroy the many-state picture?

There has been some controversy about the nature of the spin-glass phase of the SK model with a transverse field. Thirumalai, Li, and Kirkpatrick,[6] using the static approximation, claimed that there is a small region in the spin-glass phase where a replica-symmetric solution is stable, unlike the classical SK model with no transverse field. On the other hand, Buttner and Usadel[7] showed recently that a full treatment, which does not utilize the static approximation, predicts that the replica-symmetric solution is always unstable in the whole spin-glass phase. Furthermore, contracting both of the above, Yokota,[8] using a pair approximation, showed that the spin-glass transition temperature increases linearly with the transverse field Γ for small Γ. Finally, Ray, Chakrabarti, and Chakrabarti[9] performed some Monte Carlo simulations which tend to support the stability of the replica-symmetric solution in the spin-glass phase and Yokota's analytic result. Recently, Goldschmidt[15] obtained a solution to the infinite-ranged spin-glass model in a transverse field with p-spin interactions in the limit of large p and showed that in that case RSB is present in the entire spin-glass phase.

In order to clarify part of the above issues, we tackle the model analytically and obtain the first-step RSB solution. In this Letter, we report results for the quenched free energy and the phase diagram. Our result for the phase diagram disagrees with the results of Yokota[8] and Ray *et al.*[9]

The Hamiltonian for N interacting spins in a transverse field Γ reads

$$\mathcal{H} = -\sum_{i<j}^{N} J_{ij}\sigma_i^z\sigma_j^z + \Gamma\sum_i^N \sigma_i^x , \qquad (1)$$

where the spins i and j are connected by the random-coupling bond J_{ij} which is Gaussian distributed with zero mean and variance J^2/N. The σ's are the Pauli spin matrices and Γ is the transverse field. The problem can be mapped into a classical spin system plus an extra "Trotter" dimension using the Trotter-Suzuki formula[16,17] with the effective classical Hamiltonian for the Mth approximant given by

$$\mathcal{H}_{\text{eff}} = -\frac{1}{M}\sum_{k=1}^{M}\sum_{i<j}^{N} J_{ij}S_{ik}S_{jk} - \frac{B}{\beta}\sum_{k=1}^{M}\sum_{i=1}^{N} S_{ij}S_{ik+1} - \frac{MNC}{\beta}, \qquad (2)$$

where we define

$$B \equiv \tfrac{1}{2}\ln\coth(\beta\Gamma/M),\qquad C \equiv \tfrac{1}{2}\ln[\tfrac{1}{2}\sinh(2\beta\Gamma/M)]. \qquad (3)$$

$S_{ik} = \pm 1$ is the classical Ising spin on the lattice (i,k), where $k = 1,2,\ldots,M$ is a label for the Trotter direction and satisfies the periodic boundary condition. Ultimately the limit $M \to \infty$ must be taken. The replica trick is then used to calculate the quenched free energy per site. After some algebra, we obtain

$$\beta f = \lim_{n\to 0}\frac{\beta^2J^2}{4nM^2}\left[\sum_{a\neq a'}\sum_{kk'}(Q_{kk'}^{aa'})^2 + \sum_a\sum_{k\neq k'}(R_{kk'}^a)^2\right] + \frac{\beta^2J^2}{4M} - \frac{1}{n}\ln\mathrm{Tr}\,e^G, \qquad (4)$$

where $a = 1,2,\ldots,n$ is the replica index and

$$G = \sum_a\sum_{k=1}^{M}(BS_k^aS_{k+1}^a + C) + \frac{\beta^2J^2}{2M^2}\left[\sum_{a\neq a'}\sum_{kk'}Q_{kk'}^{aa'}S_k^aS_{k'}^{a'} + \sum_a\sum_{k\neq k'}R_{kk'}^aS_k^aS_{k'}^a\right]. \qquad (5)$$

The Q's and R's satisfy the saddle-point equations

$$Q_{kk'}^{aa'} = \frac{\mathrm{Tr}\,S_k^aS_{k'}^{a'}e^G}{\mathrm{Tr}\,e^G}\quad (a\neq a'),\qquad R_{kk'}^a = \frac{\mathrm{Tr}\,S_k^aS_{k'}^ae^G}{\mathrm{Tr}\,e^G}\quad (k\neq k'). \qquad (6)$$

Because of the translational invariance in the Trotter direction, the order parameters depend on $|k-k'|$. We will assume the Q's to be static, i.e., independent of $|k-k'|$, but not the R's. This assumption can be understood from the nature of $Q^{aa'}$, which is the order parameter in the spin-glass phase, and was further supported by a numerical investigation[7] of the saddle-point equations of the Q's. Also, it will be shown later that this is a self-consistent assumption. It has been shown, without assuming $R_{kk'}$ to be static, that the replica-symmetric (RS) solution is unstable[7] in the whole spin-glass phase. Thus the RSB solution must be considered in order to describe the spin-glass phase correctly. We use Parisi's scheme of RSB as in the case of the SK model. $R_{kk'}^a$ has a single replica index and is replica symmetric. For $Q^{aa'}$, we use first-step RSB with a parametrized as $a = (K,\gamma)$, where $K = 1,2,\ldots,n/m$ is the box label and $\gamma = 1,2,\ldots,m$ is the label inside a box. The values of $Q^{aa'}$ are classified according to the number of replica indices in the same box. The possible values are Q_2 and Q_{11}. After some algebra, we obtain the expression for f,

$$\beta f = \frac{\beta^2J^2}{4}\left[m(Q_2^2 - Q_{11}^2) - Q_2^2 + \frac{1}{M^2}\sum_{k\neq k'}R_{|k-k'|}{}^2 + \frac{1}{M}\right] - \frac{1}{m}\int Dz\ln\int Dy\,Z_H^m, \qquad (7)$$

where $Dz \equiv (dz/\sqrt{2\pi})\exp(-z^2/2)$ and $Z_H \equiv \mathrm{Tr}\,e^H$ with H being the new Hamiltonian of M Ising spins τ,

$$H = \frac{\beta^2J^2}{2M^2}\sum_{k,k'}(R_{kk'} - Q_2)\tau_k\tau_{k'} + B\sum_{k=1}^{M}\tau_k\tau_{k+1} + \frac{\beta J}{M}(z\sqrt{Q_{11}} + y\sqrt{Q_2 - Q_{11}})\sum_{k=1}^{M}\tau_k + MC, \qquad (8)$$

and the periodic boundary condition is obeyed. Q_{11}, Q_2, and $R_{|k-k'|}$ satisfy the saddle-point equations that extremize f,

$$Q_{11} = \int Dz\left[\frac{\int Dy\langle\tau_k\rangle_H Z_H^m}{\int Dy\,Z_H^m}\right]^2,\qquad Q_2 = \int Dz\frac{\int Dy\langle\tau_k\rangle_H^2 Z_H^m}{\int Dy\,Z_H^m},\qquad R_{|k-k'|} = \int Dz\frac{\int Dy\langle\tau_k\tau_{k'}\rangle_H Z_H^m}{\int Dy\,Z_H^m}\quad (k\neq k'), \qquad (9)$$

where $\langle\cdots\rangle_H \equiv \mathrm{Tr}(\cdots e^H)/Z_H$. If one assumes $R_{kk'}$ to be static, then the $M\to\infty$ limit can be taken analytically and we obtain the free-energy density at first-step RSB,

$$\beta f = \frac{\beta^2J^2}{4}[m(Q_2^2 - Q_{11}^2) - Q_2^2 + R^2] - \frac{1}{m}\int Dz\ln\int Dy\left[\int Dw\,2\cosh[\beta(\Gamma^2+\phi^2)^{1/2}]\right]^m, \qquad (10)$$

where $\phi \equiv w\sqrt{R - Q_2} + z\sqrt{Q_{11}} + y\sqrt{Q_2 - Q_{11}}$. However,

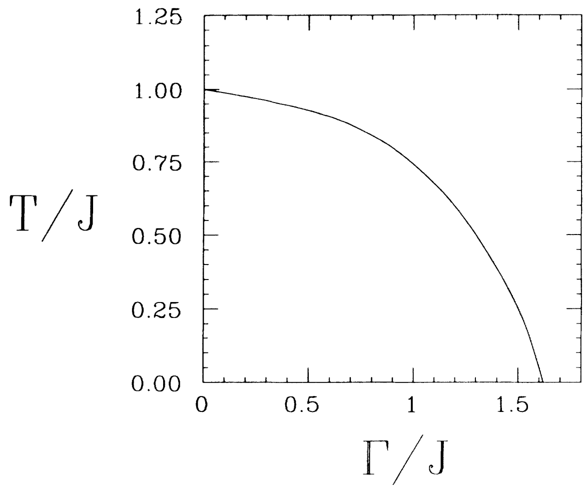

FIG. 1. Phase diagram of the Ising spin glass in a transverse field at first-step RSB.

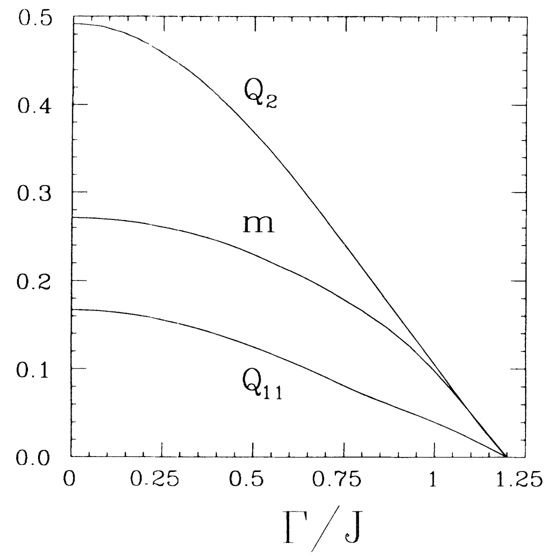

FIG. 2. Q_2, Q_{11}, and m vs Γ at $T/J=0.6$.

we now show that such an assumption is not self-consistent. The right-hand sides of the equations for Q_{11} and Q_2 in (9) are indeed independent of k since $\langle\tau_k\rangle_H$ is k independent. On the other hand, $\langle\tau_k\tau_{k'}\rangle_H$ on the right-hand size of $R_{kk'}$ depends on $|k-k'|$. Even if one assumes $R_{kk'}$ to be static in Eq. (8), $\langle\tau_k\tau_{k'}\rangle_H$ is still dependent on $|k-k'|$ unless $B=0$, implying that the static assumption on $R_{kk'}$ is not self-consistent. The Q's, R's, and m are then solved from Eqs. (9) together with the equation $\partial f/\partial m=0$, which is obtained from extremizing f. The RS case can be recovered by setting $Q_{11}=Q_2$. In practice, one needs to compute the partition function Z_H and the averages $\langle\cdots\rangle_H$. This can be done by direct spin summation if M is not too large. A Monte Carlo method can also be used to calculate the averages and the partition function.[18] In this paper, we use direct spin summation and obtain results for finite values of M and extrapolate to $M\to\infty$ using the $1/M^2$ law.[17]

For a given transverse field Γ, we obtain the values of the order parameters Q_{11} and Q_2 at different temperatures for various values of M ($M\le 8$). Our results agree very well with the $1/M^2$ law and the values at $M=\infty$ are obtained. Above the glass transition temperature $Q_{11}=Q_2=0$. As the temperature is increased, the critical temperature at which Q_2 and Q_{11} fall to zero is located. The phase diagram of the glass transition temperature versus Γ is then produced. As shown in Fig. 1, the phase diagram is in qualitative agreement with the one obtained with the RS solution in the high-temperature phase[5] without using the static approximation. The critical field above which no glass transition occurs is about $1.6J$. Our result disagrees with the prediction by Yokota[8] and recent Monte Carlo simulation results[9] which indicate the glass transition temperature increases with Γ for small Γ. Pair approximation has been used in Yokota's analysis, which we anticipate to be the reason for the discrepancy. For the Monte Carlo work, the size of the systems simulated is small ($N=32$) and the error bars are too large to allow any firm conclusion. We have also performed Monte Carlo simulations, which will be reported elsewhere,[19] for larger system sizes, and the phase boundary obtained is in agreement with Fig. 1.

To demonstrate that the RSB solution is the correct solution in the spin-glass phase, we display in Fig. 2 the variation of Q_2 and Q_{11} as a function of Γ at $T/J=0.6$. In the spin-glass phase ($\Gamma/J<1.2$), $Q_2>Q_{11}>0$ and RS is indeed broken. Figure 3 shows the free energy as

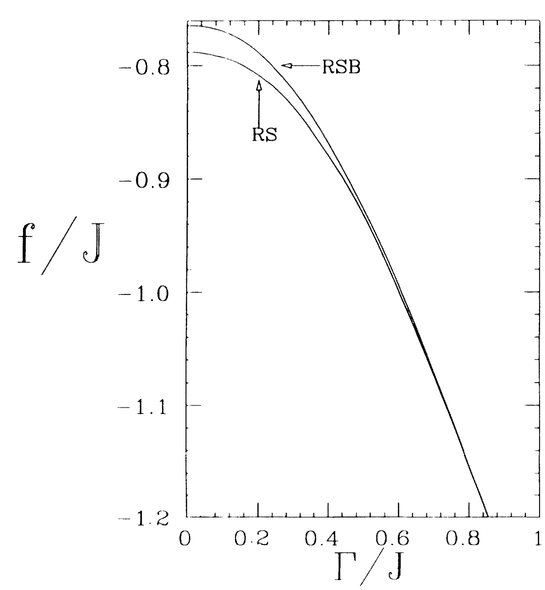

FIG. 3. Free-energy density vs the transverse field at $T/J=0.1$. First-step RSB and replica-symmetric solutions are shown.

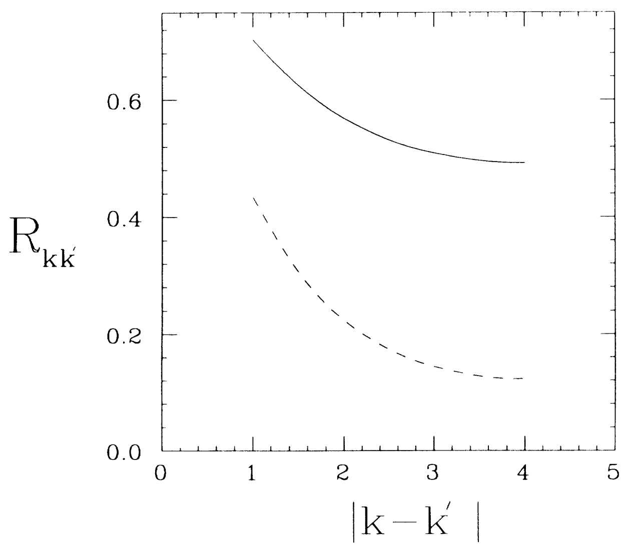

FIG. 4. $R_{kk'}$ vs $|k-k'|$. Solid line: $T/J=0.4$, $\Gamma/J=1.0$, spin-glass phase. Dashed line: $T/J=0.4$, $\Gamma/J=1.6$, paramagnetic phase.

a function of Γ at $T/J=0.1$ for the RS and RSB solutions. The RSB solution always has a higher free energy than the RS solution in the spin-glass phase, indicating that RS is broken. (In the $n\rightarrow 0$ limit in the replica trick, one maximizes the free energy rather than minimizing it.) No indication is found to support an intermediate phase[6] with spin-glass ordering and RS, in agreement with the results of Ref. 7. Finally, to illustrate that the static approximation is indeed not correct, we show in Fig. 4 $R_{kk'}$ as a function of $|k-k'|$ in the spin-glass and paramagnetic phases. In both phases, $R_{kk'}$ is a decreasing function of $|k-k'|$.

The present method can be extended to construct a higher-step RSB solution for this model. We expect the changes in the free energy to be relatively small as in the classical case.[14]

To conclude, we obtained the solution of the infinite-range Ising spin glass in a transverse field with first-step RSB. We find that, though suppressed by quantum effect, the spin-glass phase still exists and replica symmetry is broken. The phase space is characterized by many almost-degenerate thermodynamic states, qualitatively similar to the classical case.

This work was supported by National Science Foundation under Grant No. DMR-8709704.

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