

Replica symmetry breaking in the transverse-field Ising spin-glass model: Two fermionic representations

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(Received 10 November 2004; revised manuscript received 11 April 2005; published 19 July 2005)

We analyze the infinite range Ising spin glass in a transverse-field Γ below the critical temperature by a one step replica symmetry breaking theory. The set of n replicas is divided in r blocks of m replicas each. We present results for different values of the block-size parameter m . The spin operators are represented by bilinear combinations of fermionic fields and we compare the results of two models: In the four-states (4-S) model the diagonal S_i^z operator has two unphysical vanishing eigenvalues, that are suppressed by a restraint in the two-states (2-S) model. In the static approximation we obtain qualitatively similar results for both models. They both exhibit a critical temperature $T_c(\Gamma)$ that decreases when Γ increases, until it reaches a quantum critical point at the same value of Γ_c and they are both unstable under replica symmetry breaking in the whole spin glass phase. Below the critical temperature we present results for the order parameters and free energy.

DOI: [10.1103/PhysRevB.72.014447](https://doi.org/10.1103/PhysRevB.72.014447)

PACS number(s): 75.10.Nr, 64.60.Cn, 75.10.Jm

I. INTRODUCTION

The Ising model in a transverse field is widely studied for being the simplest system of interacting spins that presents a quantum critical point (QCP).¹ We will not discuss here the extensive literature on results for several versions of the model, but we will concentrate instead on the transverse-field Ising spin-glass model in the ordered region. The experimental realizations of this model are $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ compounds.²

When the transverse field Γ vanishes, our restraint two-states (2S) model for two states reduces to the Sherrington-Kirkpatrick (SK) model of a spin glass³ that in the ordered phase presents a landscape of many almost degenerate thermodynamic states separated by huge free energy barriers. The existence of these multiple states reflects itself in the breakdown of the replica symmetric solution of the saddle point equations below the ordering temperature with the onset of the de Almeida-Thouless instability^{4,5} and its replacement by Parisi's replica symmetry breaking solution.⁶ The question is if such a picture remains true when quantum mechanical effects are included or if the quantum fluctuations will be strong enough to cause tunneling between these free energy barriers.

The nature of the spin-glass phase in the transverse-field Ising spin-glass model has been the subject of controversial results that seem to depend on the representation of the spin operators, because in the calculation of the quantum mechanical partition function special tools are needed to deal with the noncommuting operators entering the Hamiltonian. The method more currently used in the study of short-range⁷ and infinite range⁸⁻¹² spin glasses in a transverse field is the Trotter-Suzuki formula,¹³ that maps a system of quantum spins in d dimensions to a classical system of spins in $(d+1)$ dimensions, and it is suited to perform numerical studies. In Ref. 10, it was found by using the static approximation that there is a small region in the spin-glass phase where a replica symmetric (RS) solution is stable, while in Ref. 11 it is predicted without the use of the static approximation that the RS solution is unstable in the whole spin glass phase. The

instability of the RS solution in the ordered region was also obtained in Ref. 12 by analyzing a one-step replica-symmetry breaking (1S-RSB) solution, and using only partially the static ansatz.

Another way of dealing with the noncommutativity of quantum mechanical spin operators is to use Feynman's path integral formulations¹⁴⁻¹⁶ and to introduce time ordering by means of an imaginary time $0 \leq \tau \leq \beta$, where β is the inverse temperature. More recently,¹⁷ conflicting results were obtained by using the formalism in Ref. 14 with the static approximation.

A still different functional integral formulation consists in using Grassmann variables to write a field theory with an effective action where the spin operators in the Hamiltonian are expressed as bilinear combinations of fermions.^{18,19} In a previous paper we used a replica symmetric (RS) theory with the static approximation and we obtained that the RS theory is unstable⁴ in all the ordered phase.¹⁸ The advantage of the fermionic formulation is that it has a natural application to problems in condensed matter theory, where the fermion operators represent electrons that also participate in other physical processes, like the Kondo effect.²⁰

In the present paper we extend our previous results¹⁸ into the ordered phase with a 1S-RSB formulation. One problem with the spin representation is that the spin eigenstates at each site do not belong to one irreducible representation $S^z = \pm 1/2$, but they are labeled instead by the fermionic occupation numbers $n_\sigma = 0$ or 1, giving two more spurious states with $S^z = 0$. We call this the "four-states" (4S) model, and despite the presence of these two unwanted states the 4S-Ising spin-glass model describes a spin-glass transition with the same characteristics as the Sherrington-Kirkpatrick (SK) model³ in a replica symmetric theory. A way to get rid of the spurious states was introduced before by Wiethege and Sherrington²¹ for nonrandom interactions and it consists of fixing the occupation number $n_{i\uparrow} + n_{i\downarrow}$ by means of an integral constraint at every site. We refer to this as the "two states" (2S)-Ising model.

In Sec. II we analyze the 4S-Ising and 2S-Ising spin-glass models in a transverse field, within the static approximation

in a one step replica symmetric breaking (1S-RSB) theory.⁶ The static ansatz neglects time fluctuations and may be considered an approximation similar to mean field theory, that describes the singularities of the zero frequency mode.¹⁵ Numerical Monte Carlo solutions of the Bray and Moore equations indicate that the static approximation reproduces the correct results at finite temperatures.²²

When $\Gamma=0$ the static approximation reproduces the results obtained by other methods, in particular for the 2S-Ising spin-glass model we recover SK equations.³ The results in both models are very similar; they both exhibit a critical spin glass temperature $T_c(\Gamma)$ that decreases when the strength Γ of the transverse field increases, until it reaches a quantum critical point (QCP) at Γ_c , $T_c(\Gamma_c)=0$. The value of $\Gamma_c=2\sqrt{2}J$ is the same for both models and the 4S-Ising and 2S-Ising models are identical close to the QCP, where $T_c \approx 2/3(\Gamma_c - \Gamma)$. We obtained for both models that the replica symmetric solution is unstable⁴ in the whole spin-glass phase, in agreement with previous results with the Trotter-Suzuki method.¹² In Parisi's theory,⁶ the first step of RSB is achieved by dividing n replicas in r blocks of m replicas each, and taking the limit $n \rightarrow 0, r \rightarrow 0$ while keeping finite the block parameter $0 \leq m \leq 1$. The block parameter m is considered to be temperature dependent and it is determined by optimization of the free energy. In our work we release this constraint and analyze the results for fixed values of the block parameter m . We present results for the free energy, and order parameters that are consistent with Ref. 12 but not with that of Ref. 17. Numerical solutions of the saddle point equations indicate that the RSB order parameter vanishes at $T=0$. We present the model in Sec. II and we leave Sec. III for discussion.

II. MODEL AND RESULTS

The Ising spin glass in a transverse field is represented by the Hamiltonian

$$H = - \sum_{ij} J_{ij} S_i^z S_j^z - 2\Gamma \sum_i S_i^x, \quad (1)$$

where the sum is over the N sites of a lattice and J_{ij} is a random coupling among all pairs of spins, with Gaussian probability distribution

$$P(J_{ij}) = e^{-J_{ij}^2 N / 16 J^2} \sqrt{N / 16 \pi J^2}. \quad (2)$$

The spin operators are represented by auxiliary fermions fields

$$S_i^z = \frac{1}{2} [n_{i\uparrow} - n_{i\downarrow}],$$

$$S_i^x = \frac{1}{2} [a_{i\uparrow}^\dagger a_{i\downarrow} + a_{i\downarrow}^\dagger a_{i\uparrow}], \quad (3)$$

where the $a_{i\sigma}^\dagger (a_{i\sigma})$ are creation (destruction) operators with fermion anticommutation rules and $\sigma = \uparrow$ or \downarrow indicates the spin projections. The number operators $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma} = 0$ or 1 , then S_i^z in Eq. (3) has two eigenvalues $\pm 1/2$ corresponding to

$n_{i\downarrow} = 1 - n_{i\uparrow}$, and two vanishing eigenvalues when $n_{i\downarrow} = n_{i\uparrow}$.

We shall use the Lagrangian path integral formulation in terms of anticommuting Grassmann fields described in a previous publication,¹⁸ so we avoid giving repetitious details. We consider two models: the unrestrained, four-states model and also the two-states model of Wiethege and Sherrington where the number operators satisfy the restraint $n_{i\uparrow} + n_{i\downarrow} = 1$, which gives $S_i^z = \pm 1/2$, at every site.²¹

By using the integral representation for the Kronecker δ function

$$\delta(n_{j\uparrow} + n_{j\downarrow} - 1) = \frac{1}{2\pi} \int_0^{2\pi} dx_j e^{ix_j [n_{j\uparrow} + n_{j\downarrow} - 1]}, \quad (4)$$

we can express Z_{4S} and Z_{2S} , the partition function for the two models, in the compact functional integral form¹⁸

$$Z\{\mu\} = \int D(\varphi^* \varphi) \prod_j \frac{1}{2\pi} \int_0^{2\pi} dx_j e^{-\mu_j \varphi_j^* \varphi_j}, \quad (5)$$

where

$$A\{\mu\} = \int_0^\beta \left\{ \sum_{j,\sigma} \left[\varphi_{j\sigma}^*(\tau) \frac{d}{d\tau} \varphi_{j\sigma}(\tau) + \mu_j \varphi_{j\sigma}^*(\tau) \varphi_{j\sigma}(\tau) \right] - H(\varphi_{j\sigma}^*(\tau), \varphi_{j\sigma}(\tau)) \right\} \quad (6)$$

and $\mu_j = 0$ for the 4S model while $\mu_j = ix_j$ for the 2S model. We now follow standard procedures to get the configurational averaged free energy per site by using the replica formalism

$$F = - \frac{1}{\beta N} \lim_{n \rightarrow 0} \frac{Z(n) - 1}{n}, \quad (7)$$

where the configurational averaged, replicated, partition function $\langle Z^n \rangle_{c,a} = Z(n)$ becomes, after averaging over J_{ij}

$$Z(n) = \int_{-\infty}^{\infty} \prod_{\alpha\beta} dq_{\alpha\beta} e^{-N\beta^2 J^2 / 2 \sum_{\alpha\beta} q_{\alpha\beta}^2} \prod_j \left\{ \prod_{\alpha} \frac{1}{2\pi} \int_0^{2\pi} dx_{j\alpha} e^{-\mu_{j\alpha} \Lambda_j(q_{\alpha\beta})} \right\} \quad (8)$$

with the replica index $\alpha = 1, 2, \dots, n$, and

$$\Lambda_j(q_{\alpha\beta}) = \int D(\varphi_\alpha^\dagger \varphi_\alpha) \exp \left[\sum_{\alpha} A_{j\alpha} \Gamma + \beta^2 J^2 4 \sum_{\alpha\beta} q_{\alpha\beta} S_j^{z\alpha} S_j^{z\beta} \right]. \quad (9)$$

We have introduced the spinors in the Fourier representation

$$\underline{\psi}_i(\omega) = \begin{pmatrix} \varphi_{i\uparrow}(\omega) \\ \varphi_{i\downarrow}(\omega) \end{pmatrix} \quad (10)$$

and the Pauli matrices to write the spin-glass part of the action in the static approximation, where

$$S_i^z = \frac{1}{2} \sum_{\omega} \underline{\psi}^\dagger(\omega) \sigma^z \underline{\psi}(\omega) \quad (11)$$

and by introducing the inverse propagator

$$\gamma_j^{-1} = i\omega + \mu_j + \Gamma \sigma_x \quad (12)$$

we can write $A_{j\alpha\Gamma}$

$$A_{j\alpha\Gamma} = \sum_{\omega} \psi_j^{\dagger\alpha}(\omega) \gamma_j^{-1}(\omega) \psi_j^{\alpha}(\omega). \quad (13)$$

We assume a one step replica symmetry breaking (1S-RSB) solution⁶ of the saddle point equations by separating the n replicas in r groups of m replicas each

$$q_{\alpha\alpha} = q + \bar{\chi},$$

$$q_{\alpha\beta} = q + \delta \quad I\left(\frac{\alpha}{m}\right) = I\left(\frac{\beta}{m}\right),$$

$$q_{\alpha\beta} = q \quad I\left(\frac{\alpha}{m}\right) \neq I\left(\frac{\beta}{m}\right), \quad (14)$$

where q is the spin-glass order parameter, $\bar{\chi}$ is related to the static susceptibility by $\bar{\chi} = T\chi$, and δ is the RSB parameter. The notation $I(K)$ means integer part.

The sums over α in the spin part of the action produce again quadratic terms that can be linearized by introducing auxiliary fields, which makes the integration over Grassmann variables straightforward.¹⁸ In the limit $n \rightarrow 0, N \rightarrow \infty$ we obtain the result for the free energy per site for the model with $2(p+1)$ states, $p=0$, or 1

$$\begin{aligned} \beta F_p = & \frac{1}{2}(\beta J)^2 \{ [\bar{\chi} + q]^2 - [\delta + q]^2 + m[\delta^2 + 2\delta q] \} \\ & - \frac{1}{m} \int_{-\infty}^{\infty} Dz_0 \log \int_{-\infty}^{\infty} Dz_1 [2K_p(q, \bar{\chi}, \delta, z)]^m, \end{aligned} \quad (15)$$

where we introduce the standard notation $Dy = e^{-y^2/2} dy / \sqrt{2\pi}$ and

$$K_p(q, \bar{\chi}, z) = p + \int_{-\infty}^{\infty} D\xi \cosh \sqrt{\Delta} \quad (16)$$

with

$$h = J\sqrt{2qz_0} + J\sqrt{2(\bar{\chi} - \delta)}\xi + J\sqrt{2\delta}z_1, \quad (17)$$

$$\Delta = (\beta h)^2 + (\beta \Gamma)^2. \quad (18)$$

The saddle point equations for the order parameters are

$$\bar{\chi}_p = \int_{-\infty}^{\infty} Dz_0 \frac{1}{\int_{-\infty}^{\infty} Dz_1 K_p^m} \int_{-\infty}^{\infty} Dz_1 K_p^{m-1} I_{\bar{\chi}} - q_p, \quad (19)$$

$$\begin{aligned} q_p = & \int_{-\infty}^{\infty} Dz_0 \frac{1}{\left\{ \int_{-\infty}^{\infty} Dz_1 K_p^m \right\}^2} \\ & \times \left\{ \int_{-\infty}^{\infty} Dz_1 K_p^{m-1} \int_{-\infty}^{\infty} D\xi \frac{\beta h}{\sqrt{\Delta}} \sinh \sqrt{\Delta} \right\}^2, \end{aligned} \quad (20)$$

$$\begin{aligned} \delta_p = & \int_{-\infty}^{\infty} Dz_0 \frac{1}{\int_{-\infty}^{\infty} Dz_1 K_p^m} \int_{-\infty}^{\infty} Dz_1 K_p^{m-2} \\ & \times \left\{ \int_{-\infty}^{\infty} D\xi \frac{\beta h}{\sqrt{\Delta}} \sinh \sqrt{\Delta} \right\}^2 - q_p, \end{aligned} \quad (21)$$

where $h(\xi, z)$ is given in Eq. (17) and we call

$$I_{\bar{\chi}} = \int_{-\infty}^{\infty} D\xi \left\{ \frac{(\beta h)^2}{\Delta} \cosh \sqrt{\Delta} + \beta^2 \Gamma^2 \frac{\sinh \sqrt{\Delta}}{\Delta^{3/2}} \right\}. \quad (22)$$

We obtain for the de Almeida-Thouless eigenvalue⁴ and entropy in both models

$$\begin{aligned} \lambda_p^{\text{AT}} = & 1 - 2(\beta J)^2 \int_{-\infty}^{\infty} Dz_0 \left\{ \frac{\int_{-\infty}^{\infty} Dz_1 K_p^{m-1} I_{\bar{\chi}}}{\int_{-\infty}^{\infty} Dz_1 K_p^m} \right. \\ & \left. - \left(\frac{\int_{-\infty}^{\infty} Dz_1 K_p^{m-1} \int_{-\infty}^{\infty} D\xi \sinh \sqrt{\Delta} \frac{\beta h}{\sqrt{\Delta}}}{\int_{-\infty}^{\infty} Dz_1 K_p^m} \right)^2 \right\}^2, \end{aligned} \quad (23)$$

$$\begin{aligned} \frac{S}{k} = & -\frac{3}{2}(\beta J)^2 \{ [\bar{\chi} + q]^2 - [\delta + q]^2 + m[\delta^2 + 2\delta q] \} \\ & + \frac{1}{m} \int_{-\infty}^{\infty} Dz_0 \log \int_{-\infty}^{\infty} Dz_1 K_p^m \\ & - (\beta \Gamma)^2 \int_{-\infty}^{\infty} Dz_0 \frac{1}{\int_{-\infty}^{\infty} Dz_1 K_p^m} \int_{-\infty}^{\infty} Dz_1 K_p^{m-1} \int_{-\infty}^{\infty} D\xi \frac{\sinh \sqrt{\Delta}}{\sqrt{\Delta}}. \end{aligned} \quad (24)$$

The first terms of the Landau expansion of the free energy in powers of q and δ gives

$$\beta F_p = \beta F_p^0 - \frac{1}{2} D m q^2 - \frac{1}{2} D (1-m) [q + \delta]^2, \quad (25)$$

where the coefficient D is

$$D = (\beta J)^2 \left\{ 1 - 2(\beta J)^2 \left(\frac{I_{\bar{\chi}}}{K_p} \right)^2 \right\} \quad (26)$$

and the integrals are to be taken when $q = \delta = 0$. Here we consider $0 < m < 1$ a free parameter and the equations will be solved for different values of m . We observe that when $m = 1$ we recover the results without RSB and q being the SG order parameter, while for $m = 0$ we recover also the RS result, but with $q + \delta$ as order parameter in agreement with Ref. 6. The critical line is given by the solution of $D = 0$.

The numerical results for the critical temperature $T_c(\Gamma)$ were shown in Ref. 18. For large values of the transverse-field Γ the 2S model and 4S model are indistinguishable. When $\Gamma = 0$, Eqs. (15) for the free energy of the 2S model

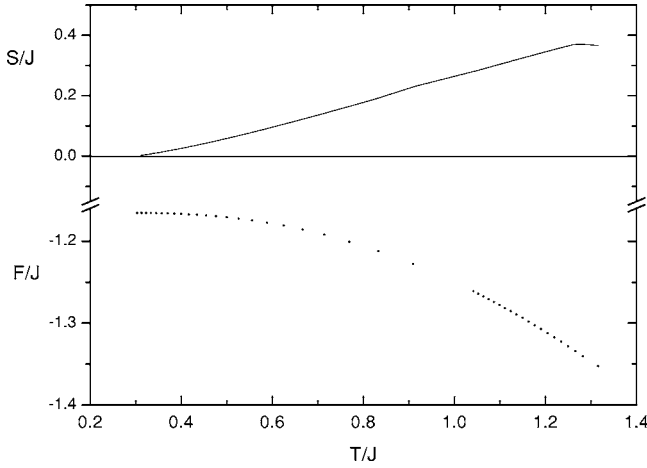


FIG. 1. Free energy and entropy for the 2S model with RSB, $m=0.8$, $\Gamma=0.5J$ as a function of temperature

($p=0$) reproduce Parisi's results for the SK model.⁶ For both models our equations coincide with Ref. 12 except for Eq. (19), because we find in our formalism that the static approximation is self-consistent. Finally, we comment on the de Almeida-Thouless instability. The numerical solution for λ^{AT} in Eq. (23) confirms that $\lambda^{\text{AT}}=0$ on the critical line $T_c(\Gamma)$ and $\lambda^{\text{AT}}<0$ for $T<T_c(\Gamma)$, indicating the instability of the replica symmetric solution in the whole ordered phase for both models and contradicting recent results in Ref. 17. We show in Fig. 1 the free energy and entropy for the 2S model ($p=0$) with RSB and $m=0.8$, $\Gamma=0.5J$. In Fig. 2 we compare the free energy for $\Gamma=0.5J$ in the 2S model with three different values of the block parameter m . In Fig. 3 we present the results for the order parameters q and δ for different values of m . In Fig. 4 we present the results for the order parameters q and δ as a function of temperature for both models in the case of RSB, with $\Gamma=0.5J$ and $m=0.8$.

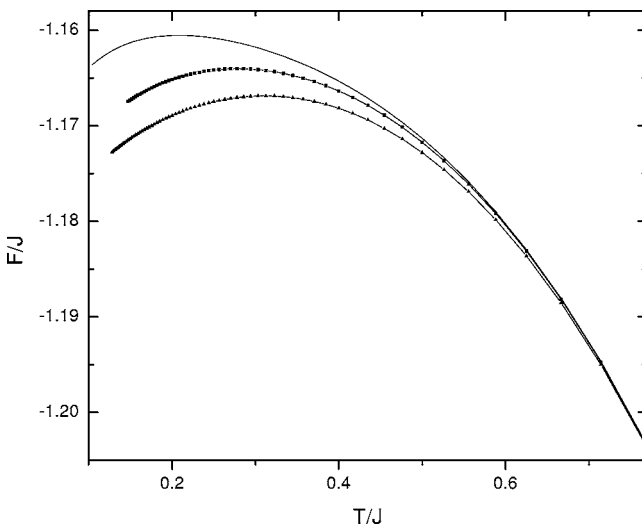


FIG. 2. Free energy for the 2S model with RSB and $m=0.2$ (full line), $m=0.4$ (squares), and $m=0.6$ (triangles), as a function of temperature for $\Gamma=0.5J$.

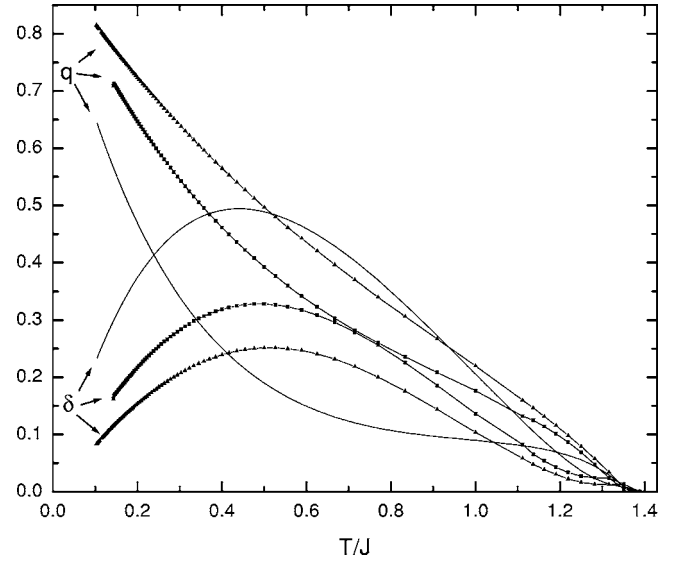


FIG. 3. Spin-glass order parameter q and RSB order parameter δ for $\Gamma=0.5J$ in the 2S model. $m=0.2$ (full line), $m=0.4$ (squares), and $m=0.6$ (triangles).

III. DISCUSSION

We apply a 1S-RSB theory⁶ to extend to low temperatures our previous study¹⁸ of two quantum Ising spin-glass models in a transverse field by means of a path integral formalism where the spin operators are represented by bilinear combinations of fermionic fields, in the static approximation. The n replicas were separated in r groups of m replicas each and we analyze the results for fixed values of the block size parameter $0 \leq m \leq 1$. This differs from Parisi's theory⁶ where m is considered to be temperature dependent and it is determined by optimization of the free energy. In the unrestricted four-states 4S model the diagonal S_i^z operator has two eigenvalues $S_i^z = \pm 1/2$ and two vanishing eigenvalues, while in the 2S model the vanishing eigenvalues are suppressed by means of an integral constraint.²¹ Regarding the de Almeida-

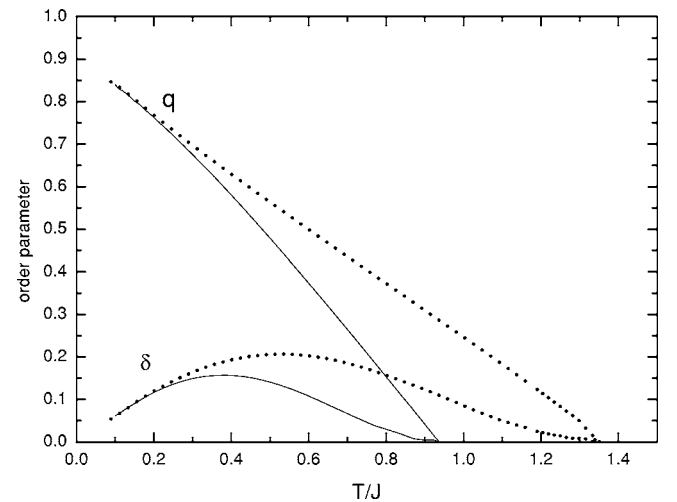


FIG. 4. Order parameters for $m=0.8$, $\Gamma=0.5J$ in the 2S model (dotted line) and 4S model (full line)

Thouless instability,⁴ we obtained before¹⁸ that the replica symmetric solution is unstable in the whole spin-glass phase for both models, contradicting the results in Ref. 17 but in agreement with the results in Refs. 11 and 12, obtained with the method of Trotter-Suzuki.¹³ The results we present here for the solutions of the saddle point equations, shown in Figs. 3 and 4, seem to indicate that the RSB order parameter δ vanishes at $T=0$ for all values of the block parameter m . The free energy, shown in Fig. 2, is maximized for smaller values of m and this is consistent with the results of Ref. 6 where it is obtained $m=0$ at $T=0$. However, if we introduce the value $\delta=0$ in our analytic expression in Eq. (24) for the entropy we would recover the RS result, in discrepancy with the numerical results of Ref. 6 at $T=0$. We believe the origin of this discrepancy lies in keeping the block parameter m fixed. We notice in Fig. 3 that for $m=0.2$ and $T \geq 0.2J$ the order parameters q and δ cross, that is $\delta \geq q$. We may conjecture that for $m=0$ this behavior extends to all temperatures $T \leq T_c$, in agreement with the numerical results.⁶

To summarize, we study the ordered phase for the Ising spin-glass model in the presence of a transverse field by using a fermionic representation of the spin operators. The RS theory is unstable for $T \leq T_c$ (Ref. 18) and we study a 1S-RSB theory where we hold fixed the block-size parameter m . We derive saddle point equations for the order parameters that agree with previous results obtained with other methods.¹² Our theory has the advantage of computational simplicity and permits us to clarify the importance of m , but it does not describe RSB at $T=0$ for finite values of $m \geq 0.2$. We conjecture that RSB is restored at $T=0$ only for $m=0$.

ACKNOWLEDGMENT

E.M.M.S. acknowledges financial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

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