Weak instability of frustrated fermionic models

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We study the Almeida-Thouless instability of two fermionic models analogous to spin glasses that exhibit frustration and that were solved some time ago with a replica symmetric ansatz. In the first model (I) we consider only the anisotropic, Ising-like limit, while in the second model (II) we consider the isotropic, Heisenberg-like Hamiltonian. In both models the interactions are of the Sherrington-Kirkpatrick type and the spins are represented by bilinear combinations of fermionic fields. While model I is almost classical, exhibiting a negative entropy at low temperatures, we show in this paper that the eigenvalue λ_{RS} is positive at the critical temperature and becomes negative at a temperature below the transition point. Model II is more interesting because λ_{RS} is positive at the critical temperature T_{SG}, vanishes at $T_1<T_{SG}$, and becomes positive again at $T_2<T_1$. Although the entropy remains positive all the way down to $T=0$, it presents a break of monotonicity when λ_{RS} becomes negative, indicating a negative specific heat in part of the instability region $T_2<T<T_1$. The two stability regions in the ordered phase for $T<T_2$ and $T_1<T<T_{SG}$ are characterized by the correct sign of the entropy and specific heat. This seems to indicate that replica symmetry stability is enhanced in frustrated fermionic spin models. [S0163-1829(97)01433-1]

I. INTRODUCTION

Since the formulation of the Sherrington-Kirkpatrick[1] (SK) theory for Ising spin glasses, a natural development followed for analogous theories with quantum spins that may exhibit interesting differences in their low-temperature properties. Spin operators form a vector in three dimensions and are a representation of the three noncommuting angular momentum operators. Hence they are quantum-mechanical quantities and the natural coupling among spins that respects rotational invariance is given by the Heisenberg model, where two spins are coupled through a scalar product. From the point of view of magnetism, the Ising model is a truncated Heisenberg model where the transverse components have been suppressed, leaving only the interaction between the components in a preferred direction. Correspondingly, say, σ_z can be considered to be diagonal with eigenvalues ± 1, and thus the Ising spin glass model is a model for ''classical'' spins. The spherical model is a generalization of the Ising model where the classical spin variables are not restricted to ± 1, but are allowed to vary continuously between $-\infty$ and ∞. Depending then on which model is going to be ''quantized,'' one obtains different theories of quantum spin glasses.

In the quantum description of the spherical model, the continuous spin variables are quantized as position variables by means of the introduction of canonically conjugated momenta.[2] This leads to a system of coupled harmonic oscillators that can be diagonalized in terms of boson operators. In a more modern version of the model,[3] the quantization procedure is done through the introduction of time dependence in the otherwise classical variables in a way analogous to the Trotter-Suzuki transformation.[4] These bosonic spin glass models exhibit positive entropy in the ordered phase down to zero temperature.

A different quantum spin glass model concerns the Ising model in a transverse field that couples to a nondiagonal spin component. In this model, the Trotter-Suzuki transformation[4] is usually used to reduce the problem to a classical one that allows it to be treated by numerical methods. Absence of replica symmetry breaking[5] in the ordered phase has been claimed[6,7] and questioned thereafter.[8]

A third line of approach considers a different quantized version of the SK model, namely, a Heisenberg analog with random long-ranged interactions and Hamiltonian

$$H=-\sum_{i,j} J_{ij}[gS_i^zS_j^z+(1-g)\tfrac{1}{2}(S_i^+S_j^-+S_i^-S_j^+)]. \quad (1)$$

The Ising[9] or extreme anisotropic limit follows for $g=1$, and the Heisenberg[10,11] or isotropic limit for $g=1/2$. In the following we indicate Refs. 9 and 10 by I and II, respectively. The random couplings J_{ij} are as in the SK model,[1] with zero mean and variance equal to $1/N$, for the system of N spins. In both papers the spin operators were represented by bilinear combinations of fermionic (anticommuting) fields[12]

$$S_i^z=\tfrac{1}{2}[\psi_{i\uparrow}^\dagger\psi_{i\downarrow}-\psi_{i\downarrow}^\dagger\psi_{i\downarrow}], \quad S_i^+=\psi_{i\uparrow}^\dagger\psi_{i\downarrow}=(S_i^-)^+. \quad (2)$$

Functional integration techniques have been known for a long time to be a powerful tool for the evaluation of the quantum-mechanical partition function. One way of implementing this is by means of the introduction of time ordering in order to treat the operators as c numbers.[11] An alternative way, which leads to applications in condensed matter theory, is the representation of spin operators by bilinear combination of fermions, since fermions may represent conduction electrons in the d band of transition metals that also contribute to the spin density. A very good introduction to this subject for the nonfamiliar reader is given in Ref. 13. A problem with this representation as it stands here, however, is that the spin eigenstates at every site do not belong to the

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same irreducible representation, but they are labeled, instead, by fermionic occupation numbers $n_{is}=0$ or 1, giving the same statistical weight to unoccupied and double occupied states.[14] In consequence of this, other properties of the $S=\frac{1}{2}$ representation are not preserved; for instance, the operator $\mathbf{S}^2$ may take the values $S(S+1)=\frac{3}{4}$ or zero. Hence we consider it more appropriate to avoid the denomination of Ising or Heisenberg and to call the Hamiltonians obtained from Eq. (1) in the limits $g=\frac{1}{2}$ or 1 of isotropic or extreme anisotropic, respectively. We also pointed out in II that the $g=1$ limit of Eq. (1) is indeed a classical problem in terms of commuting operators that does not require functional integration methods, but that in spite of this some quantum features remain in that the susceptibility χ now emerges as an order parameter because the fermionic representation allows for states with $S_i^z=\pm\frac{1}{2}$ or 0. The calculations in I were performed in a replica-symmetric (RS) theory, obtaining the expected negative entropy at very low temperatures as in the SK model.[1] In II the functional integral formalism was needed, and by using a replica-symmetric theory, we cast the problem into that of n fermions at one site with a retarded interaction in the presence of a time-dependent field. We have shown that, when the field is treated in the static approximation and the interaction in the instantaneous approximation, a mean-field description of the spin glass transition with positive entropy is obtained down to zero temperature. The Almeida-Thouless instability[5] was not analyzed either for model I or for model II.

In a more recent paper,[15] fermionic functional integration techniques in the static approximation were also used to analyze the quantum Ising spin glass model in Fock space we presented earlier in I, but in the presence of a longitudinal field. The results obtained reduce to ours[9] in zero field, but it was found that the Almeida-Thouless stability was violated everywhere in the spin glass phase for finite fields. It was this revival of interest in the problem[3,15] that motivated us to complete our previous investigations, and in the present work we analyze the replica symmetry instability of the models in I and II, in zero field, and we show that in both cases it is controlled by the replicon mode eigenvalue λ_{RS} that becomes negative at a temperature $T_1<T_{SG}$, where T_{SG} is the spin glass transition temperature. Moreover, in model II there is a second temperature $T_2<T_1$, where λ_{RS} becomes positive again, remaining positive all the way down to zero temperature. The entropy in model II remains positive for all temperatures, but part of the unphysical region with RS instability exhibits a negative specific heat.

This weakening of the RS instability in frustrated fermionic spin systems is the main result reported in this paper. We will skip here standard mathematical manipulations that are not essential for the understanding of the work, referring the reader to I and II for details. We analyze briefly in Sec. II the results for λ_{RS} in the extreme anisotropic limit[9] for completeness, since our results partly overlap with Ref. 15 and their results overlap with ours in I. We report in Sec. III original results for the isotropic model[10] in II.

II. RS INSTABILITY IN THE EXTREME ANISOTROPIC LIMIT

It was discussed in Sec. IV of II that, in the limit $g=1$, the Hamiltonian of Eq. (1) is expressed only in terms of the

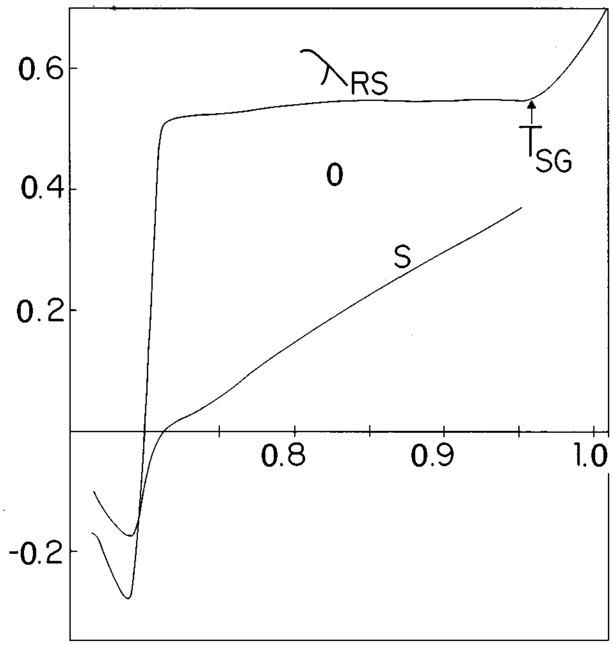

FIG. 1. Entropy (S) and replicon eigenvalue (λ_{RS}) for model I. The arrow indicates the spin glass transition temperature T_{SG}.

commuting operators S_i^z and that functional integrals are not needed, since the partition function can be obtained as the trace over the commuting occupation number operators $n_{is}=0$ or 1. Either with this method or with the method of I, the correlation functions can be calculated through differentiation by introducing replica-dependent auxiliary fields and we obtain, for the de Almeida–Thouless[5] eigenvalue,

$$\lambda_{RS}=1-\beta^2\int_0^\infty Dz\,\frac{[1+x\,\cosh(\beta\sqrt{2q}z)]^2}{[x+\cosh(\beta\sqrt{2q}z)]^4}, \tag{3}$$

where $Dz=\sqrt{(2/\pi)}e^{-(z^2)/2}dz$ and $x=e^{-\beta^2\chi}$. The spin glass order parameter q and the susceptibility χ are given by the saddle-point equations[9]

$$q=\int_0^\infty Dz\,\frac{[\sinh(\beta\sqrt{2q}z)]^2}{[x+\cosh(\beta\sqrt{2q}z)]^2}$$

$$\chi=\int_0^\infty Dz\,\frac{[1+x\,\cosh(\beta\sqrt{2q}z)]}{[x+\cosh(\beta\sqrt{2q}z)]^2}, \tag{4}$$

while the entropy is given by

$$\frac{S}{k}=-\frac{3}{2}\beta^2\chi[\chi+2q]+\int_0^\infty Dz\,\ln\left[1+\frac{1}{x}\cosh(\beta\sqrt{2q}z)\right]. \tag{5}$$

In this model, $T_{SG}=0.96$ and we find that at the critical temperature, $\lambda_{RS}=\frac{1}{2}$, while the results in Fig. 1 show that λ_{RS} and S remain positive up to $T_1\approx0.7$, indicating that there is a finite region of stability below T_{SG}. Equating λ_{RS} to zero in Eq. (3) above, one recovers the result of Ref. 15.

III. RS INSTABILITY IN THE ISOTROPIC LIMIT

When $g=\frac{1}{2}$ the Hamiltonian in Eq. (1) couples the three noncommuting components of the spin operators and we are forced to use functional integration techniques, where the introduction of time dependence allows us to treat the operators as classical variables. We chose in II to represent the spin operators in terms of fermionic Grassmann (anticommuting) fields,[12] and a very detailed comparison with other methods and previous work was presented there. We reproduce here only the essential expressions to follow the calculation of λ_{RS}.

The configurational-averaged thermodynamic potential per site of the Heisenberg model Hamiltonian reads, from Eq. (13) of I,

$$\beta\Omega=\lim_{n-0}\frac{1}{n}\left\{\frac{1}{8\beta^2}\sum_{\alpha\alpha'}\sum_{tt'}\sum_{\nu\nu'}|Q^{tt'}_{\alpha\alpha'}(\nu\nu')|^2-\ln(\Lambda)\right\}, \tag{6}$$

where Λ is an effective partition function,

$$\Lambda=\int D\{\psi^\dagger\psi\}e^A, \tag{7}$$

$$A=\sum_\alpha A^0_\alpha+\sum_{\alpha\alpha'}\sum_{tt'}\sum_{\nu\nu'}[Q^{tt'}_{\alpha\alpha'}(\nu\nu')S^t_\alpha(-\nu)S^{t'}_{\alpha'}(-\nu')], \tag{8}$$

and we indicate by α a replica index, by t a space direction x, y, or z, and by $\nu=2\pi l$ a boson Matsubara frequency. The spin operators in Eq. (8) are represented by bilinear combinations of Grassmann fields

$$S^t_\alpha(\nu)=\frac{1}{2}\sum_{s_1s_2\omega}\psi^\dagger_{s_1\alpha}(\omega+\nu)\sigma^t_{s_1s_2}\psi_{s_2\alpha}(\omega), \tag{9}$$

where $\sigma^t_{s_1s_2}$ are elements of a Pauli matrix, while the Q variables are complex fields that satisfy the saddle-point equations

$$Q^{tt'}_{\alpha\alpha'}(\nu\nu')=4\beta^2\langle S^t_\alpha(\nu)S^{t'}_{\alpha'}(-\nu')\rangle, \tag{10}$$

obtained by extremizing $\beta\Omega$ in Eq. (5). The free action in Eq. (7) is given by

$$A^0_\alpha=\sum_{\nu s}(i\omega+\mu)\psi^\dagger_{\alpha s}(\omega)\psi_{\alpha s}(\omega)-2\vec{h}'_\alpha\cdot\vec{S}_\alpha(0), \tag{11}$$

where we introduced α-dependent auxiliary fields $\vec{h}'_\alpha$ to obtain the correlation functions entering in λ_{RS} by differentiation. Following II, we parametrize the Q fields according to the ansatz

$$Q^{tt'}_{\alpha\alpha'}(\nu\nu')=4\beta^2\delta_{\nu\nu'}\delta_{tt'}\{[q+\kappa_{\alpha\alpha'}]\delta_{\nu0}+\tfrac{1}{2}\chi(\delta_{\alpha\alpha'}-1)\}, \tag{12}$$

where $\chi(\nu)=\chi$ and $q(\nu)=q\delta_{\nu0}$ are the replica-symmetric solution of II, while $\kappa_{\alpha\alpha'}$ is the replica-symmetry-breaking field. We obtain by introducing Eq. (12) into Eq. (6) and by expanding to second order in the κ variables,

$$n\beta\Omega=n\beta\Omega_{RS}+2\beta^2\left\{3\sum_{\alpha\alpha'}\kappa^2_{\alpha\alpha'}-4\beta^2\sum_{\alpha\alpha'}\sum_{\beta\beta'}\kappa_{\alpha\alpha'}\kappa_{\beta\beta'}\times\langle[\vec{S}_\alpha(0)\cdot\vec{S}_{\alpha'}(0)][\vec{S}_\beta(0)\cdot\vec{S}_{\beta'}(0)]\rangle_{cum}\right\}, \tag{13}$$

where $\beta\Omega_{RS}$ is the replica-symmetric result of II. The correlation functions in Eq. (13) are cumulant averages to be calculated from Eq. (7) in the replica symmetric theory. The replicon eigenvalue[8] is given by

$$\lambda_{RS}=3-4\beta^2[M-2N+L], \tag{14}$$

where, for $\alpha\neq\alpha'\neq\beta\neq\beta'$,

$$M=\langle[\vec{S}_\alpha(0)\cdot\vec{S}_{\alpha'}(0)]^2\rangle$$
$$N=\langle[\vec{S}_\alpha(0)\cdot\vec{S}_\beta(0)][\vec{S}_\beta(0)\cdot\vec{S}_{\beta'}(0)]\rangle$$
$$L=\langle[\vec{S}_\alpha(0)\cdot\vec{S}_{\alpha'}(0)][\vec{S}_\beta(0)\cdot\vec{S}_{\beta'}(0)]\rangle, \tag{15}$$

From Eqs. (7), (8), (11), and (61) of II, we obtain, for the correlation function of m-spin operators,

$$\langle S^t_\beta(0)S^{t'}_{\beta'}(0)\cdots(m\ \text{times})\rangle=\lim_{n\to0}\left(2^{n-m}\int D\vec{v}\frac{\partial}{\partial h^t_\beta}\frac{\partial}{\partial h^{t'}_{\beta'}}\cdots\times\exp\sum_\alpha\left\{\ln[1+\cosh|\vec{H}_\alpha|]-\frac{\eta^2_\alpha}{5\beta^2\chi}\right\}\right)_{\vec{h}'=0}, \tag{16}$$

where η_α satisfies the stationarity condition

$$\eta_\alpha=\frac{5\beta^2\chi}{2}\tanh\frac{|\vec{H}_\alpha|}{2},$$

$$\vec{H}_\alpha=\vec{h}'_\alpha+(\beta\sqrt{2q}v+\eta_\alpha)\frac{\vec{v}}{v},$$

$$\int D\vec{v}\cdots=\sqrt{\frac{2}{\pi}}\int_0^\infty dv\ v^2e^{-v^2/2}\cdots. \tag{17}$$

After solving for M, N, and L in Eq. (12), we obtain, for λ_{RS},

$$\lambda_{RS}=3-\frac{\beta^2}{4}\int D\mathbf{v}\left\{\frac{2}{h^2}\left[\tanh\frac{H}{2}\right]^2+\frac{1}{4[\cosh(H/2)]^4}\left[1+\frac{\partial\eta}{\partial h}\right]^2\right\}, \tag{18}$$

where $H=h+\eta$, $h=\beta\sqrt{2q}v$, and we obtain from II the equations for the order parameters:

$$12\chi=\int D\mathbf{v}\frac{v}{\beta\sqrt{2q}}\tanh\frac{H}{2},$$

$$12q=5\int D\mathbf{v}\left[\frac{\eta}{5\beta^2\chi}\right]^2. \tag{19}$$

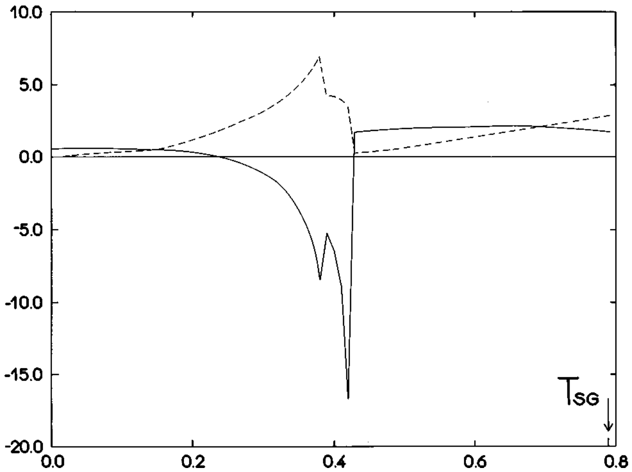

FIG. 2. Entropy (dashed line) $(0.4\times S)$ and replicon eigenvalue $(10^{-1}\lambda_{RS})$ (solid line) for model II. The arrow indicates the spin glass transition temperature T_{SG}.

The results for λ_{RS} and S are shown in Fig. 2. The exact limiting values are $\lambda_{RS}=0.6$, $S=0$ at $T=0$ and $\lambda_{RS}=1.8$, $S=1.386k_B$ at $T_{SG}=0.79$. Although the entropy remains positive at low temperatures, it has a break of monotonicity when λ_{RS} becomes negative.

IV. COMMENTS

We report in this paper results about the replica symmetry stability of two frustrated fermionic spin models,[9,10] obtained by using functional integral methods. The extreme anisotropic model discussed in Sec. II shows a region of RS stability below the transition temperature. The results for the isotropic model in Sec. III are more interesting because we can distinguish three characteristic temperatures.

(a) $T_{SG}=0.79$. For $T<T_{SG}$ we have $q\neq 0$ and $S>0$.

(b) $T_1\approx 0.42$. At this temperature, $\lambda_{RS}=0$ and $\partial S/\partial T=0$. For $T_1<T<T_{SG}$, the replica-symmetric solution is stable and the specific heat $T\ \partial S/\partial T$ is positive.

(c) $T_2\approx 0.22$, when λ_{RS} becomes positive again. For $T_2<T<T_1$, the replica-symmetric solution is unstable and does not describe the system behavior. Positiveness of the entropy is a necessary but not sufficient condition, and this region should be analyzed with a replica-symmetry-breaking solution.[16]

(d) For $T<T_2$, we have again a replica-symmetric stable solution with $\lambda_{RS}>0$ and positive entropy and specific heat.

It was also found in some models for neural networks that the stability region does not coincide with the physical region with positive values of the entropy.[17] For a different quantum model, the SK model in a transverse field, the RS stability has been analyzed by other authors using the Trotter-Suzuki transformation and numerical methods. The results are not conclusive, and while some authors[7] claim RS stability in some regions of the ordered phase, this result is contested in other works.[8] Given the difference in models and techniques, it is difficult to compare our results with the aforementioned references. In the ''Heisenberg'' model described in Ref. 15, the spin components are decoupled and the model is not rotational invariant; so a comparison with our work is out of question. Although the models discussed here have regions of stability below the critical temperature, it is known that the SK model has broken replica symmetry in the whole low-temperature phase. This is not contradictory, as discussed in Ref. 16, because this result applies only to the SK model and it does not prevent other models from behaving differently.

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[1] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975).
[2] P. Shukla and S. Singh, Phys. Lett. **81A**, 477 (1981).
[3] Th. Nieuwenhuizen, Phys. Rev. Lett. **74**, 4289 (1995).
[4] M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976).
[5] J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978).
[6] P. Ray, B. K. Chakrabarty, and Arunava Chakrabarty, Phys. Rev. B **39**, 11 828 (1989).
[7] D. Thirumalai, Li Qiang, and T. R. Kirkpatrick, J. Phys. A **22**, 3339 (1989).
[8] G. Buttner and K. D. Usadel, Phys. Rev. B **41**, 428 (1990).
[9] A. Theumann and M. Vieira Gusmão, Phys. Lett. **105A**, 311 (1984).
[10] Alba Theumann, Phys. Rev. B **33**, 559 (1986).
[11] A. J. Bray and M. A. Moore, J. Phys. C **13**, 419 (1980).
[12] K. B. Efetov, Adv. Phys. **32**, 53 (1983).
[13] D. Sherrington, in *Path Integrals*, Vol. 34 of *NATO Advanced Study Institute, Series B: Physics*, edited by G. J. Papadopoulos and J. T. Devreese (Plenum, New York, 1978).
[14] W. Wiethege and D. Sherrington, J. Phys. C **19**, 6983 (1986).
[15] R. Oppermann and X. Müller-Groening, Nucl. Phys. B **401**, 507 (1993).
[16] M. Mézard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
[17] W. Krauth and M. J. Mézard, J. Phys. (France) **20**, 3057 (1989).