Equilibrium Properties of the Ising Frustrated Lattice Gas

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Abstract. — We study the equilibrium properties of an Ising frustrated lattice gas with a mean field replica approach. This model bridges usual *Spin Glasses* and a version of *Frustrated Percolation* model, and has proven relevant to describe the glass transition. It shows a rich phase diagram which in a definite limit reduces to the known Sherrington-Kirkpatrick spin glass model.

1. Introduction

The Ising Spin Glass transition has been discovered to describe many seemingly different phenomena, and to model real systems much beyond what originally thought [1]. The idea of introducing frustrated Hamiltonians to capture the essential physics of glasses, random media properties, evolutionary models, protein and RNA folding, granular packing, dynamics of complex flow, and many others, has grown fertile in the last years [2–10].

Recently, in this panorama, an Ising Spin Glass like model, a general version of the frustrated lattice gas, has been introduced for its new interesting Monte Carlo dynamical and equilibrium features relevant to the description of the glass transition [6,7], and with some variations has been applied in the context of phase transitions in granular packing [8].

In this paper we study the mean field equilibrium properties of such a model, adopting standard replica formalism. The system we consider is characterized by the following Hamiltonian:

$$\mathcal{H} = J \sum_{\langle ij \rangle} (1 - \varepsilon_{ij} S_i S_j) n_i n_j - \mu \sum_i n_i - h \sum_i S_i n_i \tag{1}$$

where the lattice gas site variables $n_i = 0, 1$ have an Ising internal degree of freedom $S_i = \pm 1$ and $\langle ij \rangle$ denotes summation over all nearest-neighbor pairs of sites. The $\varepsilon_{ij} = \pm 1$ are quenched random variables, h is a magnetic field applied on the system and μ is a chemical potential for the site variables. Essentially, the model considers a lattice gas in a frustrated medium where the particles have an internal degree of freedom (given by its spin) that accounts, for example, for possible orientations of complex molecules in glass forming liquids. As stressed by

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Coniglio [6], these steric effects are greatly responsible for the geometric frustration appearing in glass forming systems at low temperatures or high densities. As is detailed in reference [7], this model offers a clear and intuitive picture of the mechanism leading to a glass transition, qualitatively reproducing the complex dynamical behaviour present in this regime.

The presented Hamiltonian is a natural bridge between *Frustrated Percolation* [6] and standard *Ising Spin Glasses* (SG). Indeed, this two apparently different models are obtained in two definite limits of its parameters. If $\mu \to \infty$ and $J/\mu \to 0$, for energetical reasons each site must be filled and the known Ising Spin Glass is obtained; on the contrary if $J \to \infty$ and $\mu/J \to 0$, generally even at $T = 0$ the configuration with each site filled is impossible. In this last limit only site configurations which do not close "frustrated loops", *i.e.* loops of filled sites whose spins are not satisfying all mutual interactions, are allowed. This corresponds to a site Frustrated Percolation in which clusters have a further weight factor of 2^{N_c} (N_c is the number of clusters in the system). Moreover, introducing clusters à la Kasteleyn and Fortuin, this Hamiltonian may be described in terms of a site-bond correlated and frustrated percolation.

With a simple transformation, $\tau_i \equiv S_i n_i$, this model may be changed into an Ising spin-1 Blume-Emery-Griffiths model (BEG) [11] in which only the bilinear coupling is affected by the quenched disorder ε_{ij}, while the spin biquadratic term has a coupling with opposite sign in relation to the original BEG model [12] (in notation of [12], $K/J = -1$) and no disorder. In the case without frustration ($\varepsilon_{ij} = 1$), that has also been studied in [12], the order parameters are the diluted magnetization $m = \langle Sn \rangle$ and the particles density $d = \langle n \rangle$. In the $\mu \to \infty$ limit one recovers the Ising model, with $d = 1$. In mean field, at $T = 0$, $d = m = \Theta(\mu)$ if $\mu \neq 0$ and $d = m = 1/3$ for $\mu = 0$. This point with density $0 < d < 1$ will become an interval when frustration is introduced. Moreover, expanding for small m we obtain the equation satisfied by the critical temperature

$$\frac{J}{T_c} = 1 + \exp\left(1 - \frac{\mu}{T_c}\right) \tag{2}$$

and one can see that this transition line is reentrant [12], effect that will also disappear when introducing frustration.

In the following sections we study the replica mean field theory of Hamiltonian (1) with a Gaussian distributed coupling. The phase diagram of the model presents several interesting regions depending on the values of T and μ/J. For highly negative values of μ/J, there is only a paramagnetic phase. Lowering the temperature at small negative values of μ/J, the system has a discontinuous transition to a spin glass phase, in which even at zero temperature the density is lower than one. Increasing μ/J, the spin glass transition becomes continuous, while the zero temperature density is still below one. This occurs up to a certain point where the density becomes unity (at $T = 0$) signalling that we are approaching the Sherrington-Kirkpatrick limit. The Parisi replica symmetry breaking solution seems to hold whenever a spin glass transition is encountered.

2. Mean Field Results

We present in this section results obtained in the mean field approximation. The starting point is the calculation of the free energy f according with the replica trick [1]:

$$\beta f = -\lim_{n \to 0} \frac{\ln[Z^n]_{\text{av.}}}{nN} \tag{3}$$

where $[\ldots]_{\mathrm{av.}}$ stands for the average over the disorder, which we suppose Gaussian with zero mean and variance J^2/N. We obtain:

$$\beta f = \lim_{n \to 0} \frac{1}{n} \left\{ \frac{\beta^2 J^2}{2} \sum_{a<b} q_{ab}^2 + \frac{\beta J}{2} \left(\frac{\beta J}{2} - 1 \right) \sum_a d_a^2 - \ln \mathrm{Tr}_{\{n^a, S^a\}} \mathrm{e}^{-\beta \mathcal{H}_{\mathrm{eff}}} \right\} \tag{4}$$

where the single site Hamiltonian is:

$$\mathcal{H}_{\mathrm{eff}} = -\beta J^2 \sum_{a<b} q_{ab} S^a n^a S^b n^b - J \left(\frac{\beta J}{2} - 1 \right) \sum_a d_a n^a - \mu \sum_a n^a - h \sum_a S^a n^a. \tag{5}$$

The self consistent equations for the order parameters are given by the saddle points of f and read:

$$q_{ab} = \langle S^a n^a S^b n^b \rangle \tag{6}$$

$$d_a = \langle n^a \rangle \tag{7}$$

where the average is done using the effective Hamiltonian. The overlap q_{ab} has a certain degree of dilution in respect to the parameter introduced in the SK model [17] and reduces to it in the limit $d_a = 1$.

2.1. REPLICA SYMMETRY. — To get a general qualitative picture of the phase diagram of the system, we first made a simple replica symmetric (RS) assumption, that is, $q_{ab} = q(1 - \delta_{ab})$ and $d_a = d$. The free energy then reads:

$$\beta f_{\mathrm{s}} = -\frac{1}{4} \beta^2 J^2 (q^2 - d^2) - \frac{1}{2} \beta J d^2 - \ln 2 - \int \mathcal{D}z \, \ln \left[1 + \mathrm{e}^{\Xi} \cosh(\beta J \sqrt{q} z + \beta h) \right] \tag{8}$$

where the Gaussian measure is $\mathcal{D}z \equiv \dfrac{\mathrm{d}z}{\sqrt{2\pi}} \mathrm{e}^{-z^2/2}$ and

$$\Xi \equiv \frac{\beta^2 J^2}{2}(d - q) + \beta(\mu - Jd) \tag{9}$$

The saddle point equations obeyed by the order parameters are:

$$d = \int \mathcal{D}z \, \frac{\cosh(\beta J \sqrt{q} z + \beta h)}{\mathrm{e}^{-\Xi} + \cosh(\beta J \sqrt{q} z + \beta h)} \tag{10}$$

and

$$q = \int \mathcal{D}z \, \frac{\sinh^2(\beta J \sqrt{q} z + \beta h)}{[\mathrm{e}^{-\Xi} + \cosh(\beta J \sqrt{q} z + \beta h)]^2}. \tag{11}$$

The effects introduced by the magnetic field will in general not be considered here and in what follows we take, unless mentioned, $h = 0$.

To characterize the system, in Figure 1 we present some representative curves for both q and d for several values of μ/J. For large values, the system approaches the SK limit ($T_{\mathrm{c}} \to J$, $d \to 1$ and $q \to q_{\mathrm{SK}}$). For $\mu/J > -0.56$, the system has a continuous transition ($q \sim 0$) at T_{c} satisfying

$$\frac{J}{T_{\mathrm{c}}} = 1 + \exp\left(1 - \frac{J}{2T_{\mathrm{c}}} - \frac{\mu}{T_{\mathrm{c}}} \right) \tag{12}$$
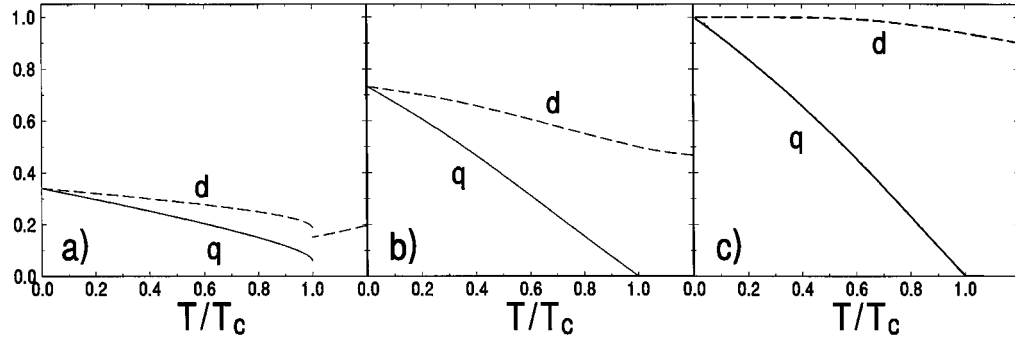
Fig. 1. — The order parameters q and d for several values of $\mu = -0.65$ (a), 0 (b) and 3 (c). Notice the diverse behaviour of d (and q) as $T \to 0$ and the discontinuous transition in (a). The respective critical temperatures are $T_c \simeq 0.13$ (a), 0.5 (b) and 0.94 (c).
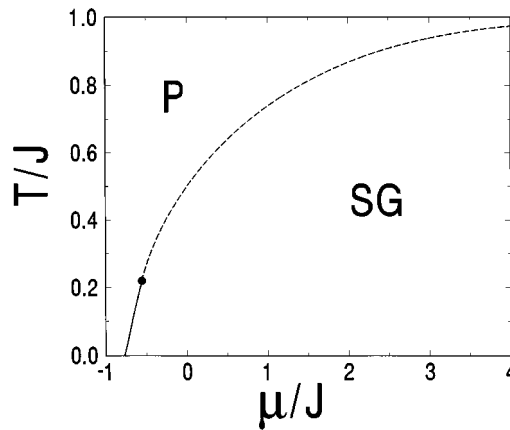

Fig. 2. — The phase diagram T *versus* μ. The dashed line stands for the continuous transition while the solid line corresponds to the first order one $(-0.77 < \mu < -0.56)$ and both meet at a tricritical point. In particular, when $J = -2\mu$, $T_c = J(1 + e)^{-1} \simeq 0.27J$ and when $\mu = 0$, $T_c = J/2$.

value to be compared with equation (2). Decreasing μ/J further, the transition line becomes first order (for $-0.77 < \mu/J < -0.56$) as signaled by a jump in the order parameter. At the transition line a partial freezing takes place ($q < d < 1$), behaviour that has to be compared with other disordered models with discontinuous transitions like, for instance, the p-states Potts glass with $p > 4$ [14] and the p-spin interaction model with $p > 2$ [15]. We can also see from Figure 1 that at low temperature q approaches d, while the actual value they assume at $T = 0$, where $q = d$ (the system being fully frozen), depends on the chemical potential as can be seen in Figure 3. The point where the transition changes behavior ($\mu/J \simeq -0.56$) turns out to be a tricritical one when including a non zero magnetic field. The system is a simple paramagnet ($q = 0$) below this region. This information is summarized in the phase diagram T *versus* μ presented in Figure 2. The reentrant phase found in the case without frustration [12] is replaced here by these various regions.
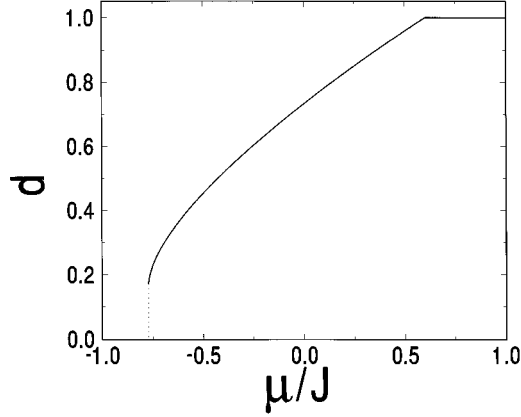
Fig. 3. — The density d *versus* μ at $T = 0$. The point for which $d \to 1$ is $\mu = 1 - (2\pi)^{-1/2}$ while for $\mu < \mu_c \simeq -0.77$ there is only the $d = 0$ solution.

It is interesting to study the $T = 0$ limit of this model. For μ above the point

$$\frac{\mu^*}{J} = 1 - \frac{1}{\sqrt{2\pi}} \simeq 0.6 \tag{13}$$

it is possible to see that $d = 1$ and $C \equiv \beta J(d-q) = \sqrt{2/\pi}$, results known to be characteristic of the Sherrington-Kirkpatrick SG. Something changes below μ^*, equation (13), where the saddle point equations give:

$$d = \operatorname{erfc}\left(\frac{-\frac{1}{2}C + d - \frac{\mu}{J}}{\sqrt{2d}}\right) \tag{14}$$

$$C = \sqrt{\frac{2}{d\pi}} \exp\left[-\frac{\left(-\frac{1}{2}C + d - \frac{\mu}{J}\right)^2}{2d}\right] \tag{15}$$

These equations imply $d < 1$ at $T = 0$, as it should be in the true $J \to \infty$ limit. On the other hand, below $\mu_c \simeq -0.77$, just the paramagnetic solution $q = d = 0$ is present, the transition being discontinuous (see Fig. 3), in accordance with the above phase diagram. The main novelties present in the model appear in this region where the chemical potential is sufficiently low and frustrated loops are not completely occupied ($d < 1$). The appearance of this region is an effect introduced by the disorder since in the no frustrated case, it reduces to the point $\mu = 0$.

The entropy per site is

$$s = \frac{1}{2}\beta^2 J^2(q^2 - d^2) + \frac{1}{2}\beta J d^2 - \beta\mu d - \beta f_s \quad . \tag{16}$$

As $T \to \infty$, $s \to 2\ln 2$ since our phase space has 4^N possible states, and at $T = 0$:
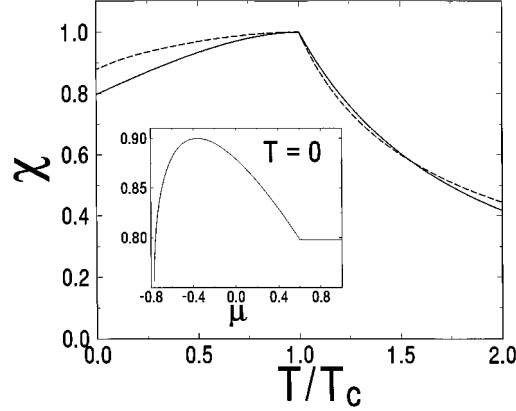
$$s_0 = -\frac{1}{4}C^2 + (1 - d)\ln 2 \quad . \tag{17}$$

Fig. 4. — The magnetic susceptibility χ *versus* T for $\mu = 0$ and 3 in RS. Inset: $T = 0$ susceptibility as a function of μ, showing a constant value above μ^* and a maximum in the region where $d(T = 0) < 1$.

For $\mu > \mu^*$, $s_0 = -1/2\pi$, while for $d = 0$, $s_0 = \ln 2$. Here we clearly see the signal of instability of the replica symmetric solution. The next section treats the first step of replica symmetric breaking in the Parisi scheme, leading to corrections to these results. We also obtain the point where $s_0 = 0$, that is, $\mu_0 \simeq -0.026$. The reason which makes positive the replica symmetric entropy below this value is the presence of free spins when the density is lower than unity. In those sites where $n_i = 0$, the spins are free to assume any orientation, and this increases the entropy (second term in Eq. (17)). The free energy hessian eigenvalues have to be calculated in order to verify the stability of the replica symmetry solution. Doing so we obtain from the condition of positive eigenvalues, the AT line [18]

$$\frac{1}{\beta^2 J^2} > \int \mathcal{D}z \, \frac{\left[1 + e^{-\Xi} \cosh(\beta J \sqrt{q}z)\right]^2}{\left[e^{-\Xi} + \cosh(\beta J \sqrt{q}z)\right]^4} \tag{18}$$

below which the replica symmetric solution is unstable. It can be verified that the above equation is satisfied nowhere below T_c and, as in the SK model, here too the replica symmetric solution is unstable, although the "degree of stability" may vary with μ.

The susceptibility, $\chi = \beta(d - q)$, presents a cusp at T_c, as can be seen in Figure 4. The zero temperature value of χ, $\chi_0 = C/J$, depends on μ as shown in the inset of Figure 4. Above μ^* it has a constant value, while below it presents a maximum. As expected above T_c, $\chi = d/T$, depending just on the density. We might have chosen to apply h to all spins in equation (1) whether their sites were occupied or not ($h \sum_i S_i$). In this case in the region where $d(T = 0) < 1$, the low temperature susceptibility (now $\chi = \beta(1 - q)$) would diverge as T^{-1} due to the free spins which have a strong response even to a weak field.

We report here the values of other quantities in order to characterize the system and for comparison with the known SG. The internal energy per spin is

$$u = \frac{1}{2}\beta J^2(q^2 - d^2) + \frac{J}{2}d^2 - d\mu \tag{19}$$

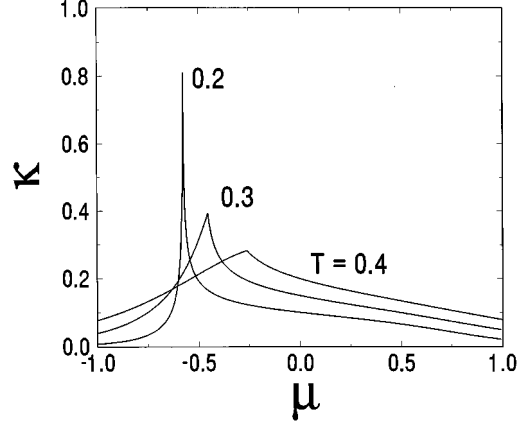and, at $T = 0$,

$$u_0 = -JCd + \frac{J}{2}d^2 - d\mu \ .$$

Fig. 5. — The compressibility κ as a function of μ/J for $T = 0.4$, 0.3 and 0.2. In the first two cases the transition is continuous and κ presents a cusp while in the last one it has a divergence since the transition is discontinuous.

The compressibility $\kappa = \beta^{-1}\partial d/\partial\mu$ has a cusp when the transition is continuous, although presents a divergence when the transition is first order, as can be seen in Figure 5.

2.2. REPLICA SYMMETRY BREAKING. — Results in the previous section have shown the instability of the RS solution and we report here the first Parisi correction to it. However, it will appear that the phase diagram sketched above in RS is not altered.

Following the Parisi scheme [1], in the first step of replica symmetry breaking (1RSB) the n replicas are divided in n/m blocks containing m replicas. Different replicas in the same block have overlap q_1 while those in different blocks have overlap q_0. Thus, the 1RSB free energy is:

$$\beta f_1 = -\frac{1}{4}\beta^2 J^2 \left[(1-m)q_1^2 + mq_0^2 - d^2\right] - \frac{1}{2}\beta J d^2$$
$$- \ln 2 - \frac{1}{m}\int \mathcal{D}z_0 \, \ln \int \mathcal{D}z_1 \, A^m(z_0, z_1) \qquad (20)$$

where:

$$A(z_0, z_1) \equiv 1 + e^{\Xi_1}\cosh(\beta h + \beta J z_0 \sqrt{q_0} + \beta J z_1 \sqrt{q_1 - q_0})$$
$$\Xi_1 \equiv \frac{\beta^2 J^2}{2}(d - q_1) + \beta(\mu - Jd).$$

As usual in spin-glass theory, we have to maximize the free energy as a function of q, d and m, and the saddle point equations are:

$$d = 1 - \int \mathcal{D}z_0 \, [A^{-1}]_A \qquad (21)$$

$$q_0 = \int \mathcal{D}z_0 \, [B]_A^2 \qquad (22)$$

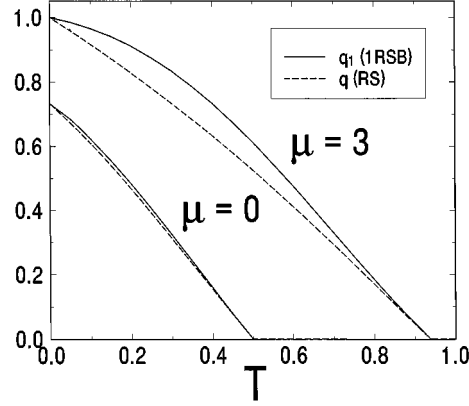$$q_1 = \int \mathcal{D}z_0 \, [B^2]_A \qquad (23)$$

Fig. 6. — The order parameter q_1 obtained with 1RSB and q with RS for $\mu = 0$ and 3. Regarding d, we did not find any difference between the RS and 1RSB solutions, while for q_1, the correction is small.

$(d \geq q_1 \geq q_0)$ and m satisfies

$$\frac{1}{4}m^2\beta^2 J^2(q_1^2 - q_0^2) - m\int \mathcal{D}z_0\,[\ln A]_A + \int \mathcal{D}z_0\,\ln\int \mathcal{D}z_1\,A^m = 0. \tag{24}$$

Here we have defined:

$$B(z_0, z_1) \equiv \frac{\sinh(\beta h + \beta J z_0 \sqrt{q_0} + \beta J z_1 \sqrt{q_1 - q_0})}{e^{-\Xi_1}A(z_0, z_1)} \tag{25}$$

and

$$[X]_A = \frac{\int \mathcal{D}z_1\,A^m X}{\int \mathcal{D}z_1\,A^m}\ . \tag{26}$$

The numerical solutions, which can be obtained by either maximizing the free energy or by solving the coupled system of saddle point equations, are shown in Figure 6. The density does not change in relation to the replica symmetric case, while the effect of replica symmetry breaking on q_1 is rather small, like in the SK model. For m, the behavior is analogous to the one found by Parisi in the SK model, $m = 0$ at both $T = 0$ and $T = T_c$, and have a maximum at an intermediate temperature.

In analogy with the SK model, the difference between f_s and f_1 is only perceptible at low temperatures, although depending on the value of μ, this effect becomes more difficult to notice. It can also be seen that $f_1 \geq f_s$, as expected, and that the regions with wrong curvature (negative entropy) in the RS solution are largely reduced.

The susceptibility is given by

$$\chi = \beta[d + (m - 1)q_1 - mq_0] \tag{27}$$

and the results of 1RSB are higher than the ones found in RS (see Fig. 4), as in the SK model. We have also checked that, at $T = 0$, the point where the density becomes lower than one coincides with the one obtained with replica symmetry, equation (13).

Our calculations in 1RSB confirm that the structure of the phase diagram found in replica symmetry is not altered when breaking it. The first order transition is quite similar to the one

found in other spin glass models [13–16], although the model deserves a more detailed study to clarify whether the transition is or not exactly described by one step of replica symmetry breaking. In this case the glassy behavior of the model could be rather peculiar and different from other disordered system with discontinuous transition.

3. Summary and Conclusions

In brief, we have studied the mean field theory of a simple spin glass version of the Blume-Emery-Griffiths model with standard replica formalism. This model, described by the Hamiltonian (1), bridges the usual SG, which is obtained in the limit $(J/\mu \to 0, \mu \to \infty)$, and a version of "frustrated percolation", which is recovered if $(\mu/J \to 0, J \to \infty)$.

We have seen that the introduction of site variables n_i enrich the phase diagram of the spin glass. Specifically we have shown that the SG phase around the "frustrated percolation" limit, i.e. $\mu/J = 0$, has peculiarities signaled, for instance, by a site density below one even in the $T = 0$ limit. Moreover, a discontinuous transition appears for negative enough values of μ/J, which may be relevant to the description of the structural glass transition [2]. These two effects, namely the broad $d < 1$ region around $\mu = 0$ and the discontinuous transition, are not present in the unfrustrated model where a reentrant phase was present [12].

The transition is characterized by a cusp in the susceptibility, although for the compressibility there is a cusp when the transition is continuous and a divergence when it is first order. By comparing the results obtained with 1RSB with those found assuming symmetry, we see that we are already very near the true mean field behavior of the system, since the corrections introduced are small. On the other hand, a more detailed analysis should be done in the region where the transition is discontinuous in order to verify whether, as happens in other models with discontinuous transition [13–16], the 1RSB solution is exact.

The mean field results obtained here are in qualitative accordance with those found through numerical simulation for $D = 3$ [7], although a simulation for the infinite range version is still lacking and it would be welcomed.

It would be interesting to study the effect of varying the couplings parameters in Hamiltonian equation (1) [19], as done in the non frustrated case in [11,12] where qualitatively different phase diagrams are so found. Also, by introducing a non zero mean in the Gaussian distribution, it might be possible to study the appearance of the reentrant phase and tune the length of the zero temperature $0 < d < 1$ interval [19]. We expect, by the above results, that the interplay of connectivity and frustration would lead to a richer behavior than the usual spin glasses.

Acknowledgments

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