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Zero-temperature TAP equations for the Ghatak-Sherrington model

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Abstract. The zero-temperature TAP equations for the spin-1 Ghatak-Sherrington model are investigated. The spin-glass energy density (ground state) is determined as a function of the anisotropy crystal field D for a large number of spins. This allows us to locate a first-order transition between the spin-glass and paramagnetic phases within a good accuracy. The total number of solutions is also determined as a function of D.

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Recently different authors have investigated some infinite-range spin-glass models which display both continuous and first-order transitions lines [1–8]. In most cases, the first-order transition line starts at a tricritical point and extends down to $T = 0$. Within the replica approach, one should in principle locate this line according to the program proposed by Parisi [9]. However, it is easy to see that this is a very hard task, and has not been achieved so far. The difficulty has its origin in the fact that at a first-order transition at least two phases with different symmetries coexist with the same free energy but distinct order parameters. In most spin-glass models at least one of these order parameters must be obtained within an accurate numerical study of the full Parisi treatment. Another method to study disordered systems was introduced in order to avoid replicas and is widely known as TAP approach [10]. It is also well-known that this method presents another kind of numerical difficulty, since the TAP equations have an exponentially large number of solutions, most of them related to metastable states [11,12]. Nevertheless, it is possible to solve the TAP equations for the Sherrigton-Kirkpatrick (SK) model [13] and get some useful information on the nature of the spin-glass phase [14,15].

Following SK, Ghatak and Sherrington [16] introduced a generalized model to the case of integer spin $S_i = 0, \pm 1, \ldots, \pm S$ and including a crystal-field term. This model is an example of the systems mentioned in the first paragraph above. For $S = 1$ it has a first-order transition line that for some time was the object of some controversies [17–19]. Although its location is presently known within the replica-symmetric solution, it was not yet determined from a full Parisi solution. Recently, Feldmann and Oppermann [20] showed that a fermionic Ising spin glass is equivalent to the spin-1 Ghatak-Sherrington model. These authors also considered a one-step replica-symmetry breaking (1RSB) in order to locate the first-order transition line. For $T = 0$ they concluded that the transition is located at $D \approx 0.881J$, where D represents the crystal field and J^2/N the variance of the random couplings, a result already known to one of us [21]. This should be compared to the replica-symmetric result which gives $D \approx 0.899J$ [19]. In fact it results in a tedious algebra but one can show that a second step in the replica-symmetry breaking (2RSB) procedure gives $D \approx 0.880J$ [21]. Thus, one may suspect that a full Parisi treatment would give a value for D/J very close to 0.88. It is thus natural to look for an alternative treatment in order to check these results.

The TAP equations for the Ghatak-Sherrington model were already obtained a few years ago by Yokota [22]. This author did an extensive numerical study of the transition at a particular temperature, namely, $T = 0.2J$. He showed that the first-order transition should be located at $D/J = 0.85 \pm 0.05$. However, he did not search for the zero-temperature transition which turns out to be simpler to analyse. On the other hand, the TAP equations for the analogous fermionic Ising spin glass were recently obtained by Rehker and Oppermann [5]. Following [20] it is easy to see that there is an exact mapping between the corresponding equations for both models. Rehker and Oppermann [5] have numerically studied their equations

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for $T = 0$ and found that the transition line is located at $D \approx 0.8J$, without any mention to error bars. They also obtained equations which determine the number of solutions for the corresponding TAP equations at any temperature, but were unable to solve them numerically even for $T = 0$.

The purpose of the present note is twofold. Firstly, we show that carrying out a numerical study with some reasonable numbers of spins, the TAP equations for the Ghatak-Sherrington model can be used to determine the transition at $T = 0$ to a good accuracy. Secondly, we show that total number of such solutions can be determined as a function of D (or, equivalently, μ in the fermionic-glass case [5]).

We consider the Hamiltonian

$$H = -\sum_{(ij)} J_{ij} S_i S_j + D \sum_i S_i^2 \ , \tag{1}$$

where each spin S_i $(i = 1, 2, \cdots, N)$ can take the values $-1, 0$ and 1 and the summations are over all distinct pairs (i, j). The random exchange couplings J_{ij} have zero mean and variance J^2/N. According to equations (3, 4) from Yokota [22], the TAP equations for this system can be written as

$$\begin{aligned} m_i &= \frac{2\sinh(\beta h_i)}{\exp(\beta \Delta_i) + 2\cosh(\beta h_i)} \\ p_i &= \frac{2\cosh(\beta h_i)}{\exp(\beta \Delta_i) + 2\cosh(\beta h_i)} \end{aligned} \tag{2}$$

where

$$h_i = \sum_j J_{ij} m_j - \beta m_i \sum_j J_{ij}^2 (p_j - m_j^2), \tag{3}$$

and

$$\Delta_i = D - \frac{1}{2}\beta \sum_j J_{ij}^2 (p_j - m_j^2), \tag{4}$$

where m_i and p_i are thermal averages fo S_i and S_i^2, respectively.

At $T = 0$ the above equation simplify to

$$\begin{aligned} m_i &= \mathrm{sgn}(h_i)\Theta(|h_i| - D), \\ h_i &= \sum_j J_{ij} m_j, \end{aligned} \tag{5}$$

where Θ is the Heaviside step function. The energy density (in units of J) is given by

$$f = -\frac{1}{NJ} \sum_{(i,j)} J_{ij} m_i m_j + \frac{D}{NJ} \sum_i p_i, \tag{6}$$

where $p_i = m_i^2$ at $T = 0$.

In the paramagnetic phase all m_i are equal zero and so is its energy density, irrespective of D. The spin-glass solutions can be found numerically. We have used an iterative approach to search for such solutions by rewriting the magnetization equations (5) as $m_{i,n+1} = \mathcal{F}(\{m_{i,n}\})$. The criterion adopted for convergence was

$$\frac{1}{N} \sum_{i=1}^{N} |m_{i,n+1} - m_{i,n}| < 10^{-6}. \tag{7}$$

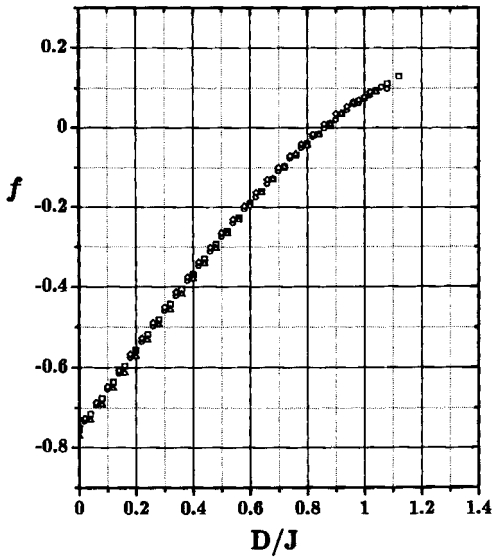

Fig. 1. Spin-glass energy density f as a function of D/J for $N = 300$ $(\triangle), 400$ $(\square), 500$ $(\diamond)$ and 600 $(\circ)$ spins. The first-order transition is located when the curves cross the horizontal zero axis, since the paramagnetic energy density is zero for any value of D.

In the present case this method works finely and allows us to obtain as many spin-glass solutions as we could. That will not be so if we were working in a non-zero temperature regime as happens in the SK model [23]. We were thus able to improve the results obtained earlier [5], analysing systems varying from a few spins up to $N = 1\,000$ spins. We have also varied the number of realizations of random interactions, N_{R}. Within each realization, the number of samples, N_{S}, was determined from distinct initial conditions obtained as spin-glass solutions of the

TAP equations for $D = 0$. For a given sample, we determine the solution with lowest energy density $f_{\min}$ at $D = 0$ and keep only solutions with energy densities such that $|f/f_{\min} - 1| < 0.05$. The solutions thus kept, typically less than 5% of N_S, are then used as initial conditions to upgrade the solutions for a new value of D. This method allows us to obtain the spin-glass energy density as a function of D for each surviving sample. Finally, we averaged over the number of surviving samples and over the number of realizations. Figure 1 summarizes our findings for the energy density. The error bars for the energy density are comparable in size to the symbols used on that figure, which give us much confidence on our results. We have also verified that for small systems (up to $N = 200$), the present method reproduces the results presented in reference [5], but with strong fluctuations. Thus, we find that the first-order transition which occurs when the spin-glass energy density becomes zero is located at

$$D/J = 0.858 \pm 0.008. \tag{8}$$

This result improves the one found previously [5]. Nevertheless, it is also remarkably different from those obtained within the replica approach [19–21]. We have no sound explanation for this discrepancy between two seemingly equivalent methods as TAP formulation and replica treatment. We hope that other methods such as Monte Carlo simulation, or exact determination of the ground state for finite systems, could help us in determining the zero-temperature transition in a definite way.

The total number of solutions to equation (5) can also be computed using the methods introduced by De Dominicis *et al.* [11] or Bray and Moore [12], and can be shown to give the same results. The latter method will be used in this note. Let us rewrite the magnetization equations as

$$m_i = \varphi(h_i), \tag{9}$$

where $\varphi(h_i) = \mathrm{sgn}(h_i)\Theta(|h_i| - D)$. We also need to introduce the Edwards-Anderson order parameter defined as

$$q = \frac{1}{N}\sum_{i=1}^{N} m_i^2. \tag{10}$$

Hence the total number of solutions $\langle N_\mathrm{s}\rangle$ is given by

$$\langle N_\mathrm{s}\rangle = N\int_0^1 \mathrm{d}q \int_{-1}^{+1}\prod_i \mathrm{d}m_i \int_{-\infty}^{+\infty}\prod_i \mathrm{d}h_i \delta(Nq - \sum_i m_i^2) \times \prod_i \left[\delta(m_i - \varphi(h_i))\left\langle \delta(h_i - \sum_{j\neq i} J_{ij}m_j)\right\rangle\right]^i, \tag{11}$$

where $\langle\mathcal{O}\rangle$ means the average of $\mathcal{O}$ over the random bonds. Introducing integral representations for the delta functions involving q and h_i in the above expression gives

$$\begin{aligned}\langle N_\mathrm{s}\rangle = N\int_0^1 \mathrm{d}q \int_{-i\infty}^{+i\infty}\frac{\mathrm{d}\lambda}{2\pi\mathrm{i}} \int_{-1}^{+1}\prod_i \mathrm{d}m_i \int_{-\infty}^{+\infty}\prod_i \mathrm{d}h_i \\ \times \int_{-\infty}^{+\infty}\prod_i \frac{\mathrm{d}y_i}{\sqrt{2\pi}}\prod_i \delta(m_i - \varphi(h_i)) \\ \times \exp\left(N\lambda q - \lambda\sum_i m_i^2 + \mathrm{i}\sum_i y_i h_i - \frac{q}{2N}\sum_i y_i^2\right) \\ \times \left\langle \exp\left(-\mathrm{i}\sum_{(ij)} J_{ij}(y_i m_j + y_j m_i)^2\right)\right\rangle.\end{aligned} \tag{12}$$

Performing the average over the Gaussian bond distribution, the last factor in (12) becomes

$$\exp\left[-\frac{J^2}{2N}\sum_{(ij)}(y_i m_j + y_j m_i)^2\right] = \exp\left[-\frac{J^2}{2N}q\sum_i y_i^2 - \frac{J^2}{2N}\left(\sum_i y_i m_i\right)^2\right], \tag{13}$$

where we have neglected terms that do not contribute in the thermodynamic limit. The final factor in (13) is simplified using the identity

$$\mathrm{e}^{-\frac{J^2}{2N}(\sum_i y_i m_i)^2} = \int_{-\infty}^{+\infty}\frac{\mathrm{d}t}{\sqrt{2\pi/N}}\mathrm{e}^{-\frac{N}{2}t^2 + \mathrm{i}Jt\sum_i y_i m_i}. \tag{14}$$

Assembling the results (13, 14) into (12), we obtain

$$\begin{aligned}\langle N_\mathrm{s}\rangle = N^{3/2}\int_0^1 \mathrm{d}q \int_{-\infty}^{+\infty}\frac{\mathrm{d}t}{\sqrt{2\pi}} \int_{-i\infty}^{+i\infty}\frac{\mathrm{d}\lambda}{2\pi\mathrm{i}} \times \int_{-1}^{+1}\prod_i \mathrm{d}m_i \\ \times \int_{-\infty}^{+\infty}\prod_i \mathrm{d}h_i \int_{-\infty}^{+\infty}\prod_i \frac{\mathrm{d}y_i}{\sqrt{2\pi}}\prod_i \delta(m_i - \varphi(h_i)) \\ \times \exp\left[-\frac{N}{2}t^2 + N\lambda q - \lambda\sum_i m_i^2 - \frac{J^2 q}{2N}\sum_i y_i^2 \right. \\ \left. + \mathrm{i}\sum_i (h_i + Jtm_i)y_i\right].\end{aligned} \tag{15}$$

In the thermodynamic limit, the above expression is dominated by the saddle point of the integrand with respect to the variables t, λ and q. Thus, we have

$$\langle N_\mathrm{s}\rangle \approx \exp\left(N\phi_T\right) \tag{16}$$

where ϕ_T is the saddle point of

$$\phi = -\frac{1}{2}t^2 + \lambda q + \ln\Xi, \tag{17}$$

and Ξ is given by

$$\Xi = 2\int_{-D/J}^{0}\frac{\mathrm{d}x}{\sqrt{2\pi}}\mathrm{e}^{-x^2/2q} + 2\int_{-\infty}^{D/J}\frac{\mathrm{d}x}{\sqrt{2\pi q}}\mathrm{e}^{-(x-Jt)^2/2q-\lambda}, \tag{18}$$

for $D > 0$. For $D \leq 0$ we recover the result for the SK model which gives $\phi_T \approx 0.1992$ [11,12,24]. Therefore, we only need to determine ϕ_T for positive values of D. This is achieved numerically solving the saddle point equations for t, λ and q. The result is presented in Figure 2. It is

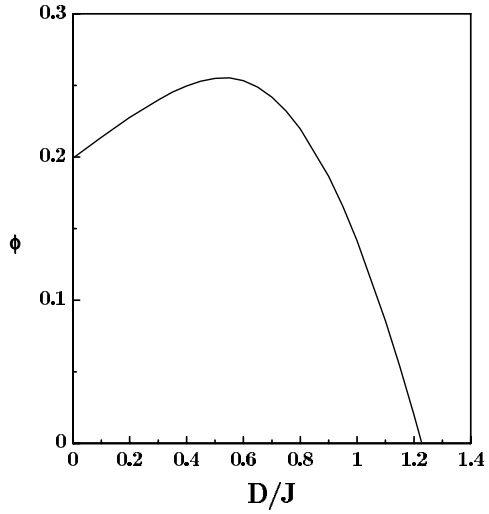

Fig. 2. The logarithm of the total number of TAP solutions per spin, $\phi_T = N^{-1}\ln\langle N_\mathrm{s}\rangle$, as a function of D/J.

interesting to note that ϕ_T has a smooth behavior as a function of D, increasing from 0.1992, reaching a maximum around $D \approx 0.550J$ and then decreasing continuously to zero at $D \approx 1.225J$. The maximum is attained when the spin-glass phase presents a large number of spins in the $S = 0$ state, whereas the remaining spins occupying the $S = \pm 1$ states are still in conflict due to frustration and randomness. Thus, the spin-glass phase may become more complex for intermediate values of D. As this parameter increases still further, eventually more and more spins prefer to stay in the $S = 0$ state and finally the paramagnetic phase becomes the unique stable phase. It is also interesting to note that in the region where the first-order transition is expected to occur the number of solutions is almost the same as in the Sherrington-Kirkpatrick model.

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