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LETTER TO THE EDITOR

The finite connectivity spin glass: investigation of replica symmetry breaking of the ground state

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Abstract. The free energy of the fixed finite connectivity spin glass is investigated in detail and we prove the equivalence of different forms which were obtained in the literature using completely different methods. Furthermore, the question of replica symmetry breaking is examined for low connectivity. We find by a variational calculation that even for a first-step breaking one can obtain a more optimal value for the ground state energy by going beyond the simple ansatz of Wong-Sherrington of totally uncorrelated groups of replicas.

There has been recent interest in the theory of randomly frustrated systems, and in particular spin glasses on lattices with finite connectivity. Such systems are closer in nature to real spin glasses because of the finite connectivity property of the lattice. In addition the spin-glass problems on random lattices with finite connectivity is closely related to some well known optimisation problems like graph partitioning and colouring [1-7].

In this letter we consider random lattices with fixed connectivity $\alpha = M+1$, for which the bonds' strength is given by a probability distribution $\rho(J)$ which is even under $J \to -J$. The lattices under consideration are random lattices which are constructed by building the connectivity matrix a_{ij}, whose elements $a_{ij} = a_{ji}$ are chosen at random to be 0 or 1 with the sole constraint

$$\sum_j a_{ij} = M+1. \tag{1}$$

Such random lattices look locally like a tree since small loops are rare [4]. They have no boundary and frustration is introduced by the existence of large loops. In addition there is numerical evidence [8, 9] that the results also apply to a Bethe lattice with 'closed' boundaries as opposed to a Bethe lattice with fixed boundary conditions which behaves differently [10].

From the point of view of application to the optimisation problem of graph partitioning it is the behaviour of the systems at $T = 0$ which is relevant and on which we will focus in this letter.

It is now becoming clear that the concept of replica symmetry breaking (RSB) has to be applied to the random lattices with finite connectivity as was previously shown to be necessary in the infinite range case [11]. The physical meaning of RSB is associated with the coexistence of many thermodynamic states separated by infinitely large free energy barriers in the thermodynamic limit. This has been established first near T_c for lattices with average finite connectivity [12], and later also for lattices with fixed finite

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connectivity [13]. Recently Goldschmidt and DeDominicis [5, 6] have shown how to systematically construct solutions with RSB at any temperature, including $T=0$ using an expansion in the inverse connectivity ($1/M$ expansion for $T>0$ and $1/\sqrt{M}$ expansion for $T=0$). The method has been used to calculate the ground state energy of spin-glass and the cost function of the graph partitioning problem for values of M as low as 9 but calculations for lower values of M requires calculation of higher orders in the large M expansion which is very tedious. The question arises whether one can directly calculate the properties of the model for small values of M. An attempt to do this was made by Wong and Sherrington (WS) [14] by using the first-step RSB approximation and by further adopting an ansatz which is equivalent to the assumption that replicas in different groups do not overlap. They showed that using this ansatz they could obtain a free energy slightly higher than that calculated using the replica symetric solution (which is an improvement since when one takes the limit $n\to 0$ in the replica method one maximises the free energy for values of $n<1$ rather than minimising it [15]).

In this letter we examine the question in greater detail. First we elucidate the relation between various expressions for free energy derived in the literature. We then show that the Wong–Sherrington ansatz is actually a stationary point of the free energy in the full space of solutions, but only for the case of a bond probability distribution of the form

$$\rho(J_{ij})=\tfrac{1}{2}\delta(J_{ij}-J)+\tfrac{1}{2}\delta(J_{ij}+J). \tag{2}$$

This is done by using the equations of motion (stationarity conditions) in a very simple form which has not been used by WS. Furthermore we show that the above stationary solution is not a true maximum for the free energy even within the framework of first-step RSB but rather one has to look for an improved solution which does not satisfy the non-overlap ansatz. This we achieve by using the variational method. We construct a trial local field distribution which depends on some variational parameters that yields a higher value for the free energy than that obtained by WS. This solution though is not a global maximum of the free energy, thus the ultimate solution for $T=0$ and finite M is not yet available. The fact that the WS solution is not the best one can also be expected from the large M calculation [5, 6] which shows that the global order parameter $g\{\sigma_k\}$ does not factorise as it does in the WS case. More on this below.

In the paper by Goldschmidt and DeDominicis [6] it has been shown how to derive an expression for the free energy of the system using the one-body and two-body density matrices, a procedure valid for a lattice having the local property of a tree. The free energy has been expressed in terms of the effective field distribution $P_n^{(M)}\{h^\alpha\}$, where $\alpha=1\ldots n$ is the replica index. h^α is the effective field exerted on a spin due to m neighbouring spins. The expression is

$$\begin{aligned} n\beta f = {} & M\ln\int\prod_\alpha \mathrm{d}h^\alpha\, P_n^{(M+1)}\{h^\alpha\}\prod_\alpha 2\cosh\beta h^\alpha \\ & -\frac{M+1}{2}\ln\int \mathrm{d}J\,\rho(J)\int\prod_\alpha \mathrm{d}h_1^\alpha\,\mathrm{d}h_2^\alpha\, P_n^{(M)}\{h_1^\alpha\}P_n^{(M)}\{h_2^\alpha\} \\ & \times\prod_\alpha\,[2\,\mathrm{e}^{\beta J}\cosh(\beta h_1^\alpha+\beta h_2^2)+2\,\mathrm{e}^{-\beta J}\cosh(\beta h_1^\alpha-\beta h_2^\alpha)]. \end{aligned} \tag{3}$$

This free energy reduces to the expressions obtained previously by Katsura *et al* [16] and Bowman and Levin [17] if one assumes replica symmetry

$$P_n^{(M)}\{h^\alpha\} = \int \mathrm{d}h\, P^{(M)}(h) \prod_\alpha \delta(h - h^\alpha). \tag{4}$$

The free energy can also be expressed in terms of the global order parameter $g_n\{\sigma^\alpha\}$ [18] which is related to the local field distribution through a Fourier transform [6]

$$g_n^M\{\mathrm{i}\sigma^\alpha\} = \int \prod_\alpha \mathrm{d}h^\alpha \exp\left(\mathrm{i}\beta \sum_\alpha h^\alpha \sigma^\alpha\right) P_n^{(M)}\{h^\alpha\} \tag{5}$$

where $\sigma^\alpha = \pm 1$ are spin variables. One can parametrise $g_n\{\sigma^\alpha\}$ in the form

$$g_n\{\sigma_\alpha\} = \sum_{r=0}^{\infty} b_r \sum_{(\alpha_1 \ldots \alpha_r)} q_{\alpha_1 \ldots \alpha_r} \sigma_{\alpha_1} \ldots \sigma_{\alpha_r} \tag{6}$$

where

$$b_r = \langle \cosh^n \beta J \tanh^r \beta J \rangle \tag{7}$$

the average being taken with respect to $\rho(J)$. Here $q_{\alpha_1 \ldots \alpha_r}$ are local order parameters. In the infinite range model only $q_{\alpha_1 \alpha_2}$ appears, but for a lattice with finite connectivity infinitely many order parameters are necessary as was first realised by Viana and Bray [12]. In terms of g_n the expression for the free energy is [5, 6]:

$$n\beta f = M \ln \mathrm{Tr}_{\sigma^\alpha} g_n^{M+1}\{\sigma_\alpha\}$$
$$- \frac{M+1}{2} \ln \int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\sigma_\alpha} \mathrm{Tr}_{\tau^\alpha} g_n^M\{\sigma_\alpha\} g_n^M\{\tau_\alpha\} \exp\left(\beta J \sum_\alpha \sigma_\alpha \tau_\alpha\right) \tag{8}$$

variation with respect to g_n yields the 'equation of motion' (stationarity condition)

$$g_n\{\sigma_\alpha\} = \mathcal{N} \int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\tau^\alpha} \exp\left(\beta J \sum \sigma_\alpha \tau_\alpha\right) g_n^M\{\tau^\alpha\} \tag{9}$$

where $\mathcal{N}$ is undetermined (the free energy does not depend on the normalisation of g_n) and we can choose it for convenience to be

$$\mathcal{N}^{-1} = \mathrm{Tr}_{\sigma_\alpha} g_n^M\{\sigma^\alpha\} \tag{10}$$

Equation (9) has been derived previously by Mottishaw [13] and the derivation is explained at length in appendix A of [6].

Note that the solution of (9) is an extremum of (8) but not necessarily a maximum. If we make use of (9) and (10) we can express the free energy (8) in a simpler form:

$$n\beta f = \tfrac{1}{2} M \ln(\mathrm{Tr}\, g_n^{M+1} / \mathrm{Tr}\, g_n^M) - \tfrac{1}{2}(\ln \mathrm{Tr}\, g_n^{M+1} + \ln \mathrm{Tr}\, g_n^M) \tag{11}$$

which has been used in the calculations of the large M expansion. ws derived [19, 14] a different expression for the free energy starting from the Viana–Bray model with the extra constraint (1).

Their expression is derived from a saddle point condition on an integral over the order parameters $q_{\alpha_1 \ldots \alpha_r}$ which is valid in the thermodynamic limit. They expressed the free energy in terms of an effective field distribution $\mathscr{P}(\{h^\alpha\})$ which is related to the order parameters via

$$q_{\alpha_1\ldots\alpha_r} = \int \prod_\alpha \mathrm{d}h^\alpha\, \mathscr{P}\{h^\alpha\} \tanh \beta h^{\alpha_r} \ldots \tanh \beta^{\alpha_r}. \tag{12}$$

Their expression for the free energy is

$$\begin{aligned} n\beta f = \frac{M+1}{2} \ln \int \mathrm{d}J\, \rho(J) \int \prod_\alpha \mathrm{d}h_1^\alpha\, \mathrm{d}h_2^\alpha\, \mathscr{P}\{h_1^\alpha\}\mathscr{P}\{h_2^\alpha\} \\ \times \cosh^n \beta J \prod_\alpha (1+\tanh \beta J \tanh \beta h_1^\alpha \tanh \beta h_2^\alpha) \\ - \ln \mathrm{Tr}_{\sigma_\alpha}\left[\int \mathrm{d}J\, \rho(J) \int \prod_\alpha \mathrm{d}h^\alpha\, \mathscr{P}\{h^\alpha\} \right. \\ \left. \times \cosh^n \beta J \prod_\alpha (1+\sigma^\alpha \tanh \beta J \tanh \beta h^\alpha)\right]^{M+1}. \end{aligned} \tag{13}$$

Let us define the function

$$G_n\{\sigma^\alpha\} = \sum_{(\alpha_1\ldots\alpha_r)} q_{\alpha_1\ldots\alpha_r}\sigma_{\alpha_1} \ldots \sigma_{\alpha_r}. \tag{14}$$

It is related to $\mathscr{P}\{h^\alpha\}$ via

$$G_n\{\mathrm{i}\sigma^\alpha\} = \int \prod_\alpha \mathrm{d}h_\alpha \exp\left(\mathrm{i}\beta \sum_\alpha h^\alpha\sigma^\alpha\right)\mathscr{P}\{h^\alpha\} \prod_\alpha \cosh^{-1}(\beta h^\alpha). \tag{15}$$

In terms of $G_n\{\sigma^\alpha\}$ the WS free energy can be written as

$$\begin{aligned} n\beta f = \frac{M+1}{2} \ln \int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\sigma^\alpha}\, \mathrm{Tr}_{\tau^\alpha} \exp\left(\beta J \sum_\alpha \sigma^\alpha\tau^\alpha\right) G\{\sigma^\alpha\}G\{\tau^\alpha\} \\ - \ln \mathrm{Tr}_{\sigma^\alpha}\left(\int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\tau^\alpha} \exp\left(\beta J \sum_\alpha \sigma^\alpha\tau^\alpha\right) G\{\tau^\alpha\}\right)^{M+1} \end{aligned} \tag{16}$$

variation of (15) with respect to G yields the equation of motion

$$X_n\{\sigma^\alpha\} = \mathscr{C} \int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\tau_\alpha} \exp\left(\beta J \sum_\alpha \sigma^\alpha\tau^\alpha\right) X_n^M\{\tau^\alpha\} \tag{17}$$

with

$$X_n\{\sigma^\alpha\} \equiv \int \mathrm{d}J\, \rho(J)\, \mathrm{Tr}_{\tau_\alpha} \exp\left(\beta J \sum_\alpha \sigma^\alpha\tau^\alpha\right) G_n\{\tau^\alpha\} \tag{18}$$

and $\mathscr{C}$ a constant independent of $\{\sigma^\alpha\}$. We see that (16) coincides with equation (9) provided we identify

$$X_n\{\sigma^\alpha\} = g_n\{\sigma^\alpha\}. \tag{19}$$

In that case

$$G_n\{\tau^\alpha\} = g_n^M\{\sigma^\alpha\} \tag{20}$$

and

$$\mathscr{P}\{h^\alpha\} = P_n^{(M)}\{h^\alpha\} \prod_\alpha \cosh \beta h^\alpha \left(\int \prod_\alpha \mathrm{d}h^\alpha P_n^{(M)}\{h^\alpha\} \prod_\alpha \cosh \beta h^\alpha\right)^{-1}. \tag{21}$$

The values of the order parameters $q_{\alpha_1\ldots\alpha_r}$ will be the same in both cases. Using (17), (19) and (20) in the expression for the free energy (16), we find that its value coincides with the previously obtained form (equation (11)). This proves that for solutions of the stationarity conditions the free energies (8) and (16) yield identical results. For values of the order parameters not satisfying the equations of motion the two free energies will differ in value. The advantage of the free energy (3) is that it is expressed in closed form in terms of the field distributions, all traces over the spins being eliminated. The expression (13) on the other hand involves traces over the spins which have to be evaluated separately for each value of M and becomes increasingly complicated for large M. Its advantage, on the other hand, comes from its derivation from the steepest descent approach. The physical acceptable solution in the thermodynamic limit must correspond to a true maximum of the free energy in the space of all order parameters. For the free energy (3) or (8) the physical solution is an extremium but not necessarily a true maximum. In the formalism leading to equation (8) stability can be checked by repeated iteration of equation (9) near its fixed point solution and finding the eigenvalues for the iterative map near that point [13]. The free energy (13) (or (16)) is the one suitable for a variational calculation since for any trial distribution (be it $G\{\sigma^\alpha\}$ or $\mathscr{P}\{h^\alpha\}$) we are guaranteed to obtain a value lower than the maximum.

Let us now take a closer look at the stationarity condition (equation (9)). In [5, 6] it has been shown how to implement a first-step RSB on that equation. Here we give only the expression in the limit of zero temperature. For 1-step breaking $g_n\{\sigma^\alpha\}$ depends only on the variables $\sigma_K = \Sigma_\gamma \sigma_{K_\gamma}$ where $\alpha = (K, \gamma)$ is the replica index and $K = 1, \ldots, n/m$; $\gamma = 1 \ldots m$. We define

$$\gamma_n\{x_K\} = g_n\{\sigma_K/\beta\} \tag{22}$$

and the equation for γ_n becomes

$$\begin{aligned}\gamma_n\{x_K\} = \mathcal{N}^{-1} \int \mathrm{d}J\,\rho(J) \int \prod_K \frac{\mathrm{d}s_K}{2\pi}\, \gamma_n^M\{\mathrm{i}s_k\} \int \prod_K \mathrm{d}u_K \exp\left(\mathrm{i}\sum s_K u_K\right) \\ \times \exp\{-\textstyle\sum x_K \operatorname{sgn} J \operatorname{sgn} u_K \min(|u_K|, |J|)\} \\ \times \exp\left\{\mu \sum_K \max(|u_K|, |J|)\right\}\end{aligned} \tag{23}$$

where

$$\mu = \lim_{\beta\to\infty} m\beta \tag{24}$$

and $\mathcal{N}$ is an appropriate normalisation [6]. It is readily seen that there is a solution of (22) of the form

$$\gamma_n\{x_K\} = \prod_K f(x_K) \tag{25}$$

provided $\rho(J)$ is of the form (2). If $\rho(J)$ is not of this form equation (25) does not constitute a solution, nor does it constitute a solution for the equation of motion in the case of average connectivity [20] even for $\rho(J)$ of the form (2). For the field distribution, equation (25) implies

$$P_n^{(M)}\{h_{K_\gamma}\} = \prod_K \int \mathrm{d}h\, P^{(M)}(h) \prod_\gamma \delta(h_{K_\gamma} - h) \tag{26}$$

where $P^{(M)}(h)$ is the Fourier transform of $[f(x)]^M$. It is then easy to verify that

$P(h) \equiv P^{(1)}(h)$ satisfies the equations

$$P(\eta) = \frac{\int \mathrm{d}h\, P^{(M)}(h) \exp\{\mu \max(|h|, 1)\}\delta(\eta - \mathrm{sgn}(h) \min(|h|, 1))}{\int \mathrm{d}\eta \exp\{\mu \max(|h|, 1)\} P^{(M)}(h)} \tag{27}$$

$$P^{(M)}(h) = \int \prod_{i=1}^{M} (\mathrm{d}\eta_i\, P(\eta_i))\delta\left(h - \sum_{i=1}^{K} \eta_i\right) \tag{28}$$

where we put for simplicity $J = 1$. For $\mu = 0$ one obtains again the equations for the case of replica symmetry [16, 17] in the limit of zero temperature.

Equations (27) and (28) have a solution of the form

$$P(\eta) = c_0\delta(\eta) + c_1(\delta(\eta + 1) + \delta(\eta - 1)) \tag{29}$$

and one can also add a continuous part as in the case of replica symmetry [16]. Of course, one can normalise $P(\eta)$ to have

$$c_0 + 2c_1 = 1. \tag{30}$$

For simplicity we restrict the subsequent discussion to the case $M = 2$. By substituting (29) in (27) and (28) we obtain the following equation for the coefficient c_0:

$$c_0 = (c_0^2 + 2c_1^2)/(c_0^2 + 2c_1^2 + 4c_0c_1 + 2c_1^2\, \mathrm{e}^{\mu}) \tag{31}$$

with c_1 given by (30).

The solution of this equation is

$$c_0 = [\mathrm{e}^{\mu} + 2 - \sqrt{(\mathrm{e}^{\mu} - 4)^2 + 8(\mathrm{e}^{\mu} - 1)}]/2(\mathrm{e}^{\mu} - 1). \tag{32}$$

Using (29) together with (28) in (3) we find

$$\begin{aligned} f = {} & \frac{2}{\mu} \ln[c_0^3 + 6c_0c_1^2 + 6\, \mathrm{e}^{\mu}(c_0^2c_1 + c_1^3) + 6\, \mathrm{e}^{2\mu}\, c_0c_1^2 + 2\, \mathrm{e}^{3\mu}\, c_1^3] \\ & - \frac{3}{2\mu} \ln[\mathrm{e}^{\mu}(c_0^2 + 2c_1^2)^2 + 8\, \mathrm{e}^{\mu}\, c_0^2c_1^2 + 8\, \mathrm{e}^{2\mu}\, c_0c_1(c_0^2 + 2c_1^2) + 8\, \mathrm{e}^{2\mu}\, c_0c_1^3 \\ & + 4\, \mathrm{e}^{3\mu}\, c_1^2(c_0^2 + 2c_1^2) + 8\, \mathrm{e}^{3\mu}\, c_0^2c_1^2 + 2\, \mathrm{e}^{3\mu}\, c_1^4 + 8\, \mathrm{e}^{4\mu}\, c_0c_1^3 + 2\, \mathrm{e}^{5\mu}\, c_1^4]. \end{aligned} \tag{33}$$

Using (33) and extremising f with respect to μ we finally find

$$f = -1.2723 \tag{34}$$

$$c_0 = 0.2971 \qquad \text{and} \qquad \mu = 0.4195. \tag{35}$$

Although we did not use a continuous part the result differs very slightly from ws who obtained $f = -1.2720$ when including a continuous part in the field distribution. We presented the details of the calculation to demonstrate how simple the present formalism is compared with the calculation of ws who did not have the explicit form (27) and (28) of the equations of motion.

One observes though that if one extremises (33) without the use of (32) one obtains (35) but this solution is not a maximum of the free energy, (the same being true for the replica symmetric solution $\mu = 0$, $c_0 = \frac{1}{3}$ which is not a maximum with respect to c_0). Actually (33) does not have an extremum which is also a maximum in the allowed range of parameters.

We also calculated the free energy (13) which for $M=2$ and $\beta\to\infty$ becomes

$$f(c_0,\mu)=\frac{3}{2\mu}\ln\int \mathrm{d}h_1\,\mathrm{d}h_2\,P_2(h_1)P_2(h_2)\exp[\mu\max(|h_1+h_2|+1,|h_1-h_2|-1)]$$
$$-\frac{1}{\mu}\ln\int\left(\prod_{i=1}^{3}\mathrm{d}h_i\,P_2(h_i)\right)\exp\left[\mu\max\left(3+\left|\sum_{i=1}^{3}h_i\right|,\sum_{i=1}^{3}|h_i|+1\right)\right] \tag{36}$$

where

$$P_2(h)=(c_0^2+2c_1^2)\delta(h)+2c_0c_1(\delta(h+1)+\delta(h-1))+c_1^2(\delta(h-2)+\delta(h+2)). \tag{37}$$

Extremising with respect to c_0 and μ we again obtained equations (34) and (35) but in this case the extremum is a maximum of (36) in the c_0, μ parameter space.

We proceed to check if the ansatz (25) is the best within the first-step RSB. In order to do that we have tried a variational global order parameter which does not have the factorisation property:

$$\gamma\{x_K\}=[(a+b\exp(\textstyle\sum x_K)+b\exp(-\sum x_K)]\prod_K(c+d\,\mathrm{e}^{x_K}+d\,\mathrm{e}^{-x_K}) \tag{38}$$

with

$$a+2b=1\qquad c+2d=1. \tag{39}$$

This form depends on three variational parameters a, c and μ. For $b=0$ we obtain the ansatz (25). For $d=0$ we obtain a replica symmetric ansatz where the field distribution is a sum of three δ-functions. The global order parameter (38) is not a solution of the equation of motion (equation (23)). Thus we use it in (13) (in the $\beta\to\infty$ limit) together with (21), where $P^{(2)}\{h^\alpha\}$ is the Fourier transform of $\gamma^2\{x_K\}$. We have found three extrema for the free energy: two of them are saddle points and correspond to the replica symmetric and to the fully factorised solution (35) respectively. The third one is a maximum and gives:

$$f=-1.271\,78\qquad \mu=0.6125\qquad a=0.682\qquad c=0.599. \tag{40}$$

Thus this free energy is higher even from the value obtained for the factorised solution with the continuous part, which suggests the true solution does not have the factorisation property. It is still a task for the future to find the ultimate solution in the first-step RBS approximation. Of course, higher-order stages of RSB will improve the result even further but their effect on the free energy is expected to be small. The result obtained from simulations of graph bi-partitioning [4] is $f=-1.260$, but one has to take into account the possible inaccuracy in the simulations, which tend to overestimate the cost function. The graph partitioning problem is *NP*-complete, thus simulation times are necessarily extremely long.

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