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Stability of the Sherrington–Kirkpatrick solution of a spin glass model

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Abstract. The stationary point used by Sherrington and Kirkpatrick in their evaluation of the free energy of a spin glass by the method of steepest descent is examined carefully. It is found that, although this point is a maximum of the integrand at high temperatures, it is not a maximum in the spin glass phase nor in the ferromagnetic phase at low temperatures. The instability persists in the presence of a magnetic field. Results are given for the limit of stability both for a partly ferromagnetic interaction in the absence of an external field and for a purely random interaction in the presence of a field.

1. Introduction

Experiments on dilute alloys of magnetic impurities in a non-magnetic metal and on other disordered or amorphous magnetic systems (see Mydosh 1977 for a review) have led to the suggestion that there is a spin glass phase of such systems, in which the spins are aligned in fixed but random directions below some critical temperature T_c. Edwards and Anderson (1975) developed a theory of the spin glass which explained some of the observed features of the spin glass phase, such as the cusp in magnetic susceptibility at T_c, but left some other features, such as the extreme sensitivity of this cusp to field strength and frequency, unexplained. For a system with energy of the form

$$H = -\sum_{(ij)} J_{ij}S_iS_j, \qquad S_i = \pm 1 \tag{1}$$

where the J_{ij} are distributed randomly, the theory is essentially a mean field theory in which the quantity

$$q = \langle\langle S_i\rangle_{\text{th}}^2\rangle_J \tag{2}$$

is studied. The thermal average of S_i at a given site is squared, and the average of this square over the distribution of the J_{ij} gives q. This work also makes use of the replica trick, in which the logarithm of the partition function Z, whose average must be calculated to find the free energy is evaluated by finding the partition function of n replicas of the system, which is Z^n, and then using the limiting process

$$\ln Z = \lim_{n\to 0} n^{-1}(Z^n - 1). \tag{3}$$

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Sherrington and Kirkpatrick (1975), which we refer to as SK, introduced a model for which one might expect mean field theory to be exact, since each of the N spins in the system was taken to interact with all the other spins. The J_{ij} were taken to be independent random variables with a common mean J_0/N and a common variance J^2/N. This choice for the N dependence of the mean and variance ensures that the energy per spin remains finite when N becomes infinite. This model appeared to be exactly solvable when the replica trick was used, and the solution reproduced many of the desirable features of the Edwards–Anderson model. However, it gave a negative entropy at low temperatures, which cannot be correct for a model with discrete Ising model spins. The authors suggested that this resulted from an improper interchange of the two limits $n\to 0$ and $N\to\infty$, and that the consequences were confined to low temperatures.

Subsequent work on this model by Thouless *et al* (1977), which avoided the replica trick confirmed that the SK solution was correct above and near T_c, but found very different behaviour at low temperatures. The differences all seem to be rdlated to the fact that the mean field on a particular spin has a normal distribution in the SK solution, but should have a different probability distribution at low temperatures. In that paper no general solution was found for intermediate temperatures, and, although the magnetic susceptibility was found, no study was made of the effect of a non-zero magnetic field.

The SK model is worth further study both because of the information it may give about the hazards of the replica trick and because a sound mean field theory is a useful starting point for more detailed theories. Harris *et al* (1976) have used renormalisation group methods for this type of problem, making use of the fact that the behaviour is supposed to be classical in six-dimensional space, and so it would be useful to understand what is contained in the 'classical' theory. Fisch and Harris (1977) have used power series methods to study the behaviour of q in a similar model in $6-\epsilon$ dimensions, and find an anomalous behaviour for 4 dimensions. This work also calls in question whether q is the right order parameter to study.

In this paper we show that there is an apparent instability in the SK solution. Not only is this instability present in the absence of an external field for all temperatures below T_c, but it exists for the non-zero field, where the SK solution is analytic. We can therefore trace out the spin glass phase boundary as a function of magnetic field. The instability also exists at low temperatures in the ferromagnetic phase, if J is non-zero. The nature of the instability suggests that the symmetry between replicas should be broken in the spin glass phase, but we have not been able to exploit this idea to calculate the properties of the spin glass phase.

2. Instability of the Sherrington–Kirkpatrick solution

By using the replica trick, Sherrington and Kirkpatrick (1975) were able to perform the averaging over the J_{ij} and the sum over sites and so express the free energy in the form

$$F=-kT\lim_{n\to 0} n^{-1}\left[\!\left[\exp\left(\frac{J^2Nn}{4(kT)^2}\right)\int\left[\prod_{(\alpha\beta)}\left(\frac{N}{2\pi}\right)^{1/2}\mathrm{d}y^{(\alpha\beta)}\right)\left(\prod_{\alpha}\left(\frac{N}{2\pi}\right)^{1/2}\mathrm{d}x^{\alpha}\right]\right.\right.$$

$$\times\exp\left\{-N\sum_{(\alpha\beta)}\frac{1}{2}y^{(\alpha\beta)2}-N\sum_{\alpha}\frac{1}{2}(x^{\alpha})^2\right.$$

$$+N\ln \operatorname{Tr}\exp\left[\frac{J}{kT}\sum_{(\alpha\beta)} y^{(\alpha\beta)}S^\alpha S^\beta+\left(\frac{J_0}{kT}\right)^{1/2}\sum_\alpha x^\alpha s^\alpha\right]\Big\}-1\Big]\tag{4}$$

where the indices α, β run from 1 to n and refer to the replica number, $(\alpha\beta)$ denotes distinct pairs with $\alpha\neq\beta$, and the trace is over the 2^n values of the $S^\alpha=\pm1$. If it is assumed that the thermodynamic limit $N\to\infty$ can be taken before the limit $n\to 0$, then the method of steepest descent can be used, and the value of the integral over the $y^{(\alpha\beta)}$ and x^α is equal to the value of the integrand where the exponent has its maximum value. This leads to the result

$$\frac{F}{N}=-\frac{J^2}{4kT}-kT\lim_{n\to0} n^{-1}\max\Big\{-\sum_{(\alpha\beta)}\frac{1}{2}y^{(\alpha\beta)2}-\sum_\alpha\frac{1}{2}x^{(\alpha)2}$$
$$+\ln \operatorname{Tr}\exp\left[\frac{J}{kT}\sum_{(\alpha\beta)} y^{(\alpha\beta)}S^\alpha S^\beta+\left(\frac{J_0}{kT}\right)^{1/2}\sum_\alpha x^\alpha S^\alpha\right]\Big\}.\tag{5}$$

There is a stationary point of the expression in braces with all x^α and $y^{(\alpha\beta)}$ zero, and this solution gives the paramagnetic phase. There may also be non-trivial stationary points given by

$$y^{(\alpha\beta)}=\frac{J}{kT}\langle S^\alpha S^\beta\rangle=\frac{Jq}{kT},$$
$$x^\alpha=\left(\frac{J_0}{kT}\right)^{1/2}\langle S^\alpha\rangle=\left(\frac{J_0}{kT}\right)^{1/2}m\tag{6}$$

where q has the same meaning as in equation (2) and m is the magnetisation, where

$$q=\frac{1}{(2\pi)^{1/2}}\int dz\,e^{-\frac{1}{2}z^2}\tanh^2\left(\frac{Jq^{1/2}}{kT}z+\frac{J_0m}{kT}\right),$$
$$m=\frac{1}{(2\pi)^{1/2}}\int dz\,e^{-\frac{1}{2}z^2}\tanh\left(\frac{Jq^{1/2}}{kT}z+\frac{J_0m}{kT}\right).\tag{7}$$

In the spin glass phase q is non-zero and m is zero, and this solution exists for $T<J/k$, while in the ferromagnetic phase m is also non-zero.

To examine the question of whether equations (6) and (7) give a maximum of the expression (5) we write

$$x^\alpha=x+\epsilon^\alpha,\qquad y^{(\alpha\beta)}=y+\eta^{(\alpha\beta)}\tag{8}$$

where x and y are the values given in equation (6), and then (5) can be expanded up to second order in the quantities ϵ^α and $\eta^{(\alpha\beta)}$. To this order the deviation of the expression in braces from its stationary value is equal to $-\frac{1}{2}\Delta$, where

$$\Delta=\sum_{\alpha,\beta}\left(\delta_{\alpha,\beta}-\frac{J_0}{kT}(\langle S^\alpha S^\beta\rangle-\langle S^\alpha\rangle\langle S^\beta\rangle)\right)\epsilon^\alpha\epsilon^\beta$$
$$+\frac{2JJ_0^{1/2}}{(kT)^{3/2}}\sum_{\delta,(\alpha\beta)}(\langle S^\delta\rangle\langle S^\alpha S^\beta\rangle-\langle S^\alpha S^\beta S^\delta\rangle)\epsilon^\delta\eta^{(\alpha\beta)}$$
$$+\sum_{(\alpha\beta),(\gamma\delta)}\left[\delta_{(\alpha\beta)(\gamma\delta)}-\left(\frac{J}{kT}\right)^2(\langle S^\alpha S^\beta S^\gamma S^\delta\rangle-\langle S^\alpha S^\beta\rangle\langle S^\gamma S^\delta\rangle)\right]\eta^{(\alpha\beta)}\eta^{(\gamma\delta)}.\tag{9}$$

This quadratic form should be positive definite for a stable solution of the problem.

The matrix $\boldsymbol{G}$ associated with this quadratic form has seven different types of matrix element. The coefficients of the ϵ have the form

$$G_{\alpha\alpha}=1-(J_0/kT)(1-\langle S^\alpha\rangle^2)=A,$$
$$G_{\alpha\beta}=-(J_0/kT)(\langle S^\alpha S^\beta\rangle-\langle S^\alpha\rangle^2)=B. \tag{10}$$

The coefficients of the η have the form

$$G_{(\alpha\beta)(\alpha\beta)}=1-(J/kT)^2(1-\langle S^\alpha S^\beta\rangle^2)=P,$$
$$G_{(\alpha\beta)(\alpha\gamma)}=-(J/kT)^2(\langle S^\beta S^\gamma\rangle-\langle S^\alpha S^\beta\rangle^2)=Q, \tag{11}$$
$$G_{(\alpha\beta)(\gamma\delta)}=-(J/kT)^2(\langle S^\alpha S^\beta S^\gamma S^\delta\rangle-\langle S^\alpha S^\beta\rangle^2)=R.$$

The cross terms have the form

$$G_{\alpha(\alpha\beta)}=G_{(\alpha\beta)\alpha}=JJ_0^{1/2}(kT)^{-\frac{3}{2}}(\langle S^\alpha\rangle\langle S^\alpha S^\beta\rangle-\langle S^\beta\rangle)=C,$$
$$G_{\gamma(\alpha\beta)}=G_{(\alpha\beta)\gamma}=JJ_0^{1/2}(kT)^{-\frac{3}{2}}(\langle S^\gamma\rangle\langle S^\alpha S^\beta\rangle-\langle S^\alpha S^\beta S^\gamma\rangle)=D. \tag{12}$$

The expectation values of spin operators that occur in these expressions are m and q, defined in equation (7), and two closely related quantities

$$t=\langle S^\alpha S^\beta S^\gamma\rangle=\frac{1}{(2\pi)^{1/2}}\int dz\, e^{-\frac{1}{2}z^2}\tanh^3\left(\frac{Jq^{1/2}}{kT}z+\frac{J_0m}{kT}\right),$$
$$r=\langle S^\alpha S^\beta S^\gamma S^\delta\rangle=\frac{1}{(2\pi)^{1/2}}\int dz\, e^{-\frac{1}{2}z^2}\tanh^4\left(\frac{Jq^{1/2}}{kT}z+\frac{J_0m}{kT}\right). \tag{13}$$

In the paramagnetic phase m, q, t and r are zero, and so the matrix is diagonal. The conditions for stability against ferromagnetism and spin glass formation are $A>0$ and $P>0$, or $kT>J_0$ and $kT>J$, in agreement with SK. For the other phases it is necessary to find the eigenvalues of the matrix. Because of the symmetry of the matrix under permutation of the indices a complete set of eigenvectors can be found for general values of n, and these are given in the appendix, so there is no problem in making the analytic continuation to $n=0$. There are at most five distinct eigenvalues. The eigenvectors that are symmetric under interchange of indices give (see equation (A.4)) for $n=0$

$$\lambda=\tfrac{1}{2}\{(A-B+P-4Q+3R)\pm[(A-B-P+4Q-3R)^2-8(C-D)^2]^{1/2}\}. \tag{14}$$

Eigenvectors that are symmetric under interchange of all but one of the indices give two more eigenvalues for general n but for $n=0$ these reduce to equation (14) (see equation (A.7)). Finally there are eigenvectors symmetric under interchange of all but two of the indices, and these give rise to the eigenvalue (see equation (A.9))

$$\lambda=P-2Q+R. \tag{15}$$

The eigenvalues given in equation (14) can be related to the free energy given by SK. Comparison of our equations (10), (11) and (12) with equations (9) and (10) of SK shows that

$$A-B=(J_0N)^{-1}\partial^2F/\partial m^2,$$
$$P-4Q+3R=-(2kT/NJ^2)\partial^2F/\partial q^2, \tag{16}$$
$$C-D=-(kT/N^2J^2J_0)^{1/2}\partial^2F/\partial m\,\partial q.$$

The condition that the product of the eigenvalues given in equation (14) is positive is equivalent to the condition that the SK solution gives a saddle point of the free energy, and this seems to be the case. We have not found any region in which the SK solution gives negative eigenvalues in equation (14), and the zeros give the phase boundaries given by SK.

The condition that the eigenvalue given by equation (15) is positive can be written in the form

$$\left(\frac{kT}{J}\right)^2 > \frac{1}{(2\pi)^{1/2}} \int \mathrm{d}z\, \mathrm{e}^{-\frac{1}{2}z^2} \operatorname{sech}^4\left(\frac{Jq^{1/2}z}{kT} + \frac{J_0 m}{kT}\right), \tag{17}$$

by using equations (11), (7) and (13). This inequality is satisfied in the paramagnetic region, where $kT > J$, but appears to be violated everywhere in the spin glass region. Close to $T = J/k$, q is small, and the inequality becomes

$$\left(\frac{kT}{J}\right)^2 > 1 - 2q\left(\frac{J}{kT}\right)^2 + 7q^2\left(\frac{J}{kT}\right)^4 - \dots \tag{18}$$

while equation (7) gives

$$q = q\left(\frac{J}{kT}\right)^2 - 2q^2\left(\frac{J}{kT}\right)^4 + \frac{17}{3}q^3\left(\frac{J}{kT}\right)^6 - \dots, \tag{19}$$

and substitution of this in (18) shows that the inequality is violated by terms of order q^2. At very low temperatures q is close to unity and the right-hand-side of the inequality (17) is of order kT/J, so it is certainly not satisfied.

In the ferromagnetic phase this inequality is satisfied for high temperatures, but it is violated at low temperatures. The line of instability obtained by numerical evaluation is shown in figure 1; it should be noticed that even for J_0 much greater than J the inequality (17) is violated at low temperatures, since for m and q close to unity and T small it gives

$$kT > \tfrac{4}{3}(2\pi)^{-1/2} J \exp(-J_0^2/2J^2). \tag{20}$$

The instability of the SK solution in this region becomes less surprising when it is noticed that the SK expression for the entropy of the ferromagnetic phase has a limit $-(Nk/2\pi)\exp(-J_0^2 m^2/J^2)$ at zero temperature. It should also be noticed that the

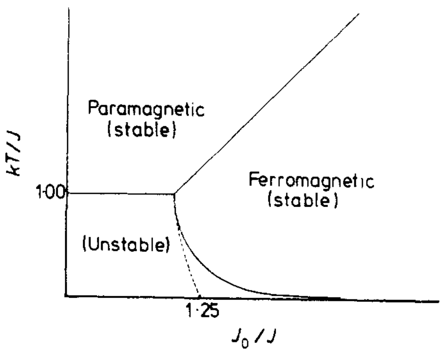

Figure 1. Phase diagram showing the limits of stability of the SK solution in the absence of a magnetic field. The broken curve is the SK phase boundary between the spin glass and ferromagnetic phases, which lies entirely in the unstable region.

instability of the ferromagnetic phase occurs for a non-zero magnetisation, and so presumably the spin glass phase can have non-zero magnetisation when J_0 is non-zero.

Very similar arguments can be applied to this system in the presence of a magnetic field. We have carried out a detailed study for the case in which J_0 is zero. The appropriate equations are obtained by replacing $J_0 m$ by H everywhere, so that the stability condition (17) and the equation for q become

$$\left(\frac{kT}{J}\right)^2 > \frac{1}{(2\pi)^{1/2}} \int dz\, e^{-\frac{1}{2}z^2} \operatorname{sech}^4\left(\frac{Jq^{1/2}z}{kT} + \frac{H}{kT}\right),$$
$$q = \frac{1}{(2\pi)^{1/2}} \int dz\, e^{-\frac{1}{2}z^2} \tanh^2\left(\frac{Jq^{1/2}z}{kT} + \frac{H}{kT}\right). \tag{21}$$

Although there is no phase transition in the SK solution for non-zero field, these equations give a line of instability for all values of the field H. For small values of H this occurs for T close to $T_c = J/k$ and q small, and a power series expansion can be used to get the condition

$$H^2 > (4J^2/3)(1 - T/T_c)^3, \tag{22}$$

while for large fields T is small and q close to unity, so that the condition becomes

$$kT > \tfrac{4}{3}(2\pi)^{-1/2} J \exp(-H^2/2J^2), \tag{23}$$

in close analogy with (20). Again it is not surprising that the SK solution should be unstable in the presence of a field, since the zero temperature limit of the entropy is $-(Nk/2\pi)\exp(-H^2/J^2)$. The result of a numerical evaluation of the line of instability given by (21) is shown in figure 2.

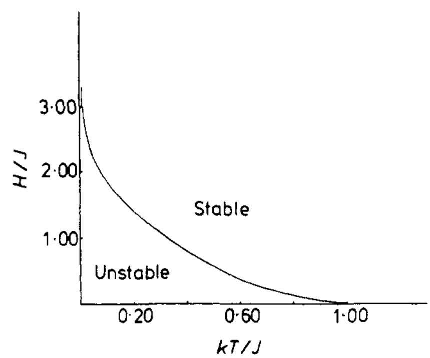

Figure 2. Phase diagram showing the limit of stability of the SK solution for the paramagnetic phase in the presence of a magnetic field H in the case $J_0 = 0$.

3. Discussion

We have shown that while at high temperatures the method used by SK to evaluate the free energy of a spin glass is consistent, in that the dominating extremum of the integrand is indeed a maximum, in the spin glass phase and in the low temperature part of the ferromagnetic phase it is not a maximum. This is consistent with the observatition made by SK that their solution must be wrong at low temperatures because their entropy is negative. This method has enabled us to trace the instability of the paramagnetic phase in a magnetic field and of the ferromagnetic phase, but we have not been able to find an alternative solution for the spin glass phase. The nature of the instability may be significant, in that it breaks the symmetry between the replicas, but it is not obvious how to handle such a broken symmetry in a zero-dimensional space.

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Appendix

To find the eigenvalues of the matrix $\boldsymbol{G}$ whose elements are given by equations (10), (11) and (12), it is necessary to exploit the symmetry of the matrix elements under permutation of the n indices. The order of the matrix is $\frac{1}{2}n(n+1)$, and since the matrix is real symmetric this is the number of linearly independent eigenvectors to be found. It turns out that by considering three symmetry classes we can find the complete set of eigenvectors and the five distinct eigenvalues.

The eigenvectors $\boldsymbol{\mu}$ of $\boldsymbol{G}$ have the form

$$\boldsymbol{\mu} = \begin{pmatrix} \{\epsilon^{(\alpha)}\} \\ \{\eta^{(\alpha\beta)}\} \end{pmatrix} \qquad \alpha, \beta = 1, 2, 3, \ldots, n \tag{A.1}$$

where $\{\epsilon^{(\alpha)}\}$ and $\{\eta^{(\alpha\beta)}\}$ are column-vectors with n and $\frac{1}{2}n(n-1)$ elements respectively. To find the solutions of the eigenvalue equation $\boldsymbol{G\mu} = \lambda\boldsymbol{\mu}$ we first consider the vector $\boldsymbol{\mu}_1$ with elements given by

$$\epsilon^{(\alpha)} = a, \qquad \text{all } \alpha; \qquad \eta^{(\alpha\beta)} = b, \qquad \text{all } (\alpha\beta). \tag{A.2}$$

Substitution of this in the eigenvalue equation gives

$$\begin{aligned} &[A+(n-1)B-\lambda]a + [(n-1)C + \tfrac{1}{2}(n-1)(n-2)D]b = 0, \\ &[2C+(n-2)D]a + [P+2(n-2)Q+\tfrac{1}{2}(n-2)(n-3)R-\lambda]b = 0, \end{aligned} \tag{A.3}$$

from which we get the two non-degenerate eigenvalues

$$\begin{aligned} \lambda = \tfrac{1}{2}[\![&[A+(n-1)B+P+2(n-2)Q+\tfrac{1}{2}(n-2)(n-3)R] \\ &\pm\{[A+(n-1)B-P-2(n-2)Q-\tfrac{1}{2}(n-2)(n-3)R]^2 \\ &+2(n-1)[2C+(n-2)D]^2\}^{1/2}]\!] \end{aligned} \tag{A.4}$$

Next we can consider the vectors $\boldsymbol{\mu}_2$ of the form

$$\begin{aligned} &\epsilon^{(\alpha)} = a, \quad \text{for } \alpha = \theta, \qquad \epsilon^{(\alpha)} = b, \quad \text{for } \alpha \neq \theta \\ &\eta^{(\alpha\beta)} = c, \quad \text{for } \alpha \text{ or } \beta = \theta, \qquad \eta^{(\alpha\beta)} = d, \quad \text{for } a, \beta \neq \theta. \end{aligned} \tag{A.5}$$

These vectors span a $2n$-dimensional invariant subspace, and therefore yield $2n$ eigenvectors, including those already obtained. To ensure orthogonality to the eigenvectors $\boldsymbol{\mu}_1$, we take $a=(1-n)b$, $c=(1-\frac{1}{2}n)d$, and the eigenvalue equation then become

$$\begin{aligned}&(A-\lambda-B)a+(n-1)(C-D)c=0,\\&\frac{n-2}{n-1}(C-D)a+[P+(n-4)Q-(n-3)R-\lambda]c=0,\end{aligned} \qquad (A.6)$$

which give two further eigenvalues

$$\begin{aligned}\lambda=\tfrac{1}{2}[\![&[A-B+P+(n-4)Q-(n-3)R]\\&\pm\{[A-B-P-(n-4)Q+(n-3)R]^2+4(n-2)(C-D)^2\}^{1/2}]\!],\end{aligned} \qquad (A.7)$$

each with degeneracy $n-1$.

Finally, the entire space can be spanned with vectors of the form

$$\begin{aligned}&\epsilon^{(\alpha)}=a, \quad \text{for } \alpha=\theta \text{ or } \nu, \qquad \epsilon^{(\alpha)}=b, \quad \text{for } \alpha\neq\theta,\nu\\&\eta^{(\theta\nu)}=c, \quad \eta^{(\theta\alpha)}=\eta^{(\nu\alpha)}=d, \quad \text{for } \alpha\neq\theta,\nu, \qquad \eta^{(\alpha\beta)}=e, \quad \text{for } \alpha,\beta\neq\theta,\nu.\end{aligned} \qquad (A.8)$$

Orthogonality to the eigenvectors already found imposes the conditions $a=b=0$, $c=(2-n)d$, $d=\frac{1}{2}(3-n)e$. Substitution of such a vector in the eigenvalue equation gives the equation

$$\lambda=P-2Q+R, \qquad (A.9)$$

with degeneracy $\frac{1}{2}n(n-3)$. These five eigenvalues are distinct in general although for $n=0$ equations (A.4) and (A.7) coincide, while for $n=1$ and $n=2$ equation (A.9) coincides with one root of (A.4) and (A.7) respectively.

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