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Parisi-like order parameter in the spherical model of a spin glass

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Abstract. An analysis of the grand canonical version of the spherical model for a spin glass (first studied by Kosterlitz, Thouless and Jones) shows that its spin glass phase can be characterized by an order parameter function. This is a consequence of the large spin length fluctuations permitted by the relaxation of the spherical constraint. Along with the distribution of order parameter values, we find a distribution function for the free energy whose variations are extensive, as well. Both distributions are reminiscent of those found in the Parisi solution and in the random energy model for the Ising spin glass. There are important differences from the solutions proposed for the Ising model. In particular, the set of overlaps does not possess an ultrametric solution.

The spherical model of a magnet with random long-range interactions, first studied by Kosterlitz, Thouless and Jones [1], is, perhaps, the simplest of the solvable models leading to a spin glass transition. As the investigation by Kosterlitz *et al* demonstrated, this model has some very useful characteristics, among them analysability with and without the use of replicas. Because of this property, the model provides a non-trivial testing ground for replication techniques as they are applied to the study of spin glass systems. One can also study other aspects of spin glass behaviour in the context of this model and obtain results that may prove to be at least suggestive regarding the behaviour of more realistic models of this system.

Kosterlitz *et al* were able to show that the replication trick and the standard assumptions that are made in applying it to spin glass systems—including replica symmetry in the ordered phase [2, 3]—yields the same results as a calculation that does not utilize replicas. The results of a subsequent study of the effects on the replica symmetric state of fluctuations indicate that the replica symmetric phase is, indeed, stable at all orders [4]. To be more precise, it was found that the ‘replicon’ models, the negative gap in whose spectrum gives rise to the deAlmeida–Thouless instability [5] in Ising and other spin glass systems, are strictly gapless in the spherical model spin glass.

The spherical model is known to be a close mathematical analogue to the ideal Bose gas of number-conserved, non-relativistic particles [6]. The spherical constraint is equivalent to the requirement of fixed particle number in the Bose gas, which is enforced in the grand canonical ensemble of that system by an adjustable chemical potential. Because of their intimate mathematical relationship the phase transitions of these two models fall into the same universality class [7]. That is to say, given identical spatial dimensionalities and a proper correspondence between spin wave and particle spectra, analogous critical exponents are the same for the two systems.

This all leads us to the following highly intriguing observation. The ideal Bose gas, in its condensed phase, displays a very interesting anomaly. In contrast to what is believed to be true of almost all other many-body systems in the thermodynamic limit, the grand canonical ensemble of the ideal Bose gas in its condensed phase is not equivalent to the canonical ensemble [8]. In particular, the occupation number of the macroscopically occupied single-particle state is not self-averaging. This number, which is $O(N)$, has fluctuations that are also $O(N)$ with finite probability as $N \rightarrow \infty$. This remarkable property of the ideal Bose gas in the grand canonical ensemble is generally dismissed as a pathology that is unique to the system, and that will disappear as soon as interactions are introduced between the particles [8, 9]. A careful study of the nature of the grand canonical ensemble, and of its relevance to real systems—even non-interacting ones—provides additional justification for ignoring this property of the ideal Bose gas [9].

We have found that the above feature of the ideal Bose gas is also present in the spherical model of the spin glass. In the case of the spherical model the two ensembles correspond to the model with the spherical constraint *strictly* enforced (the ‘strict’ spherical model) and the model with the constraint enforced *on the average* (the ‘mean’ spherical model). It is the mean spherical model that corresponds to the grand canonical ensemble, and it is on that model that we will concentrate our discussion from this point on. We stress that in relaxing the length constraint, we render the model into a different form from the strict version considered by Kosterlitz *et al*. In the strict version the order parameter *is* self-averaging. As we will see, taking the mean spherical model seriously yields, first, a Parisi-like order parameter [10, 11] and, second, a free energy distribution that bears a resemblance to the distribution of Mézard *et al* [12], but describes macroscopic rather than $O(1/N)$ fluctuations. It is hoped that further study of these tantalizing results and their consequences will lead to a deepened understanding of the spin glass phase, and that we will be taken one step closer to a complete *ab initio* characterization of spin glasses.

Given the simplicity of the spherical model, the derivation of the main results to be reported here is relatively uncomplicated and can be presented almost in its entirety. We start with the standard spin glass Hamiltonian

$$H = -\frac{1}{2} \sum J_{ij} s_i s_j \quad (1)$$

where the s_i s are scalar or Ising-like spins and the coupling strengths J_{ij} are random with a Gaussian distribution and have an infinite range. That is, $\langle J_{ij} \rangle = 0$ and $\langle (J_{ij})^2 \rangle = J^2/N$, independent of i and j [3]. The quantity N is the total number of spins in the system. The eigenvalue distribution of a real symmetric N by N matrix with independently random elements and the kind of distribution that controls the elements of the interaction matrix \mathbf{J} is given, in the limit of large N , by the well known semicircle law [13].

The spherical constraint is enforced by introducing a Lagrange multiplier into the Hamiltonian, i.e. $\beta H \rightarrow \beta H + \Lambda \sum s_i^2$. In terms of the normalized eigenfunctions of the matrix \mathbf{J} , denoted by $\psi^{(\lambda)}$, so that

$$\sum_j J_{ij} \psi_j^{(\lambda)} = \lambda \psi_i^{(\lambda)} \quad (2)$$

one has

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp\left(\frac{1}{2}\beta \sum J_{ij}s_i s_j - \Lambda \sum s_i^2\right) \prod_i ds_i$$

$$= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2} \sum_{\lambda} s^{(\lambda)^2} [2\Lambda - \beta\lambda]\right) \prod_{\lambda} ds^{(\lambda)} \quad (3)$$

where $s^{(\lambda)}$ is the amplitude of the corresponding eigenfunction.

The spin glass transition occurs when the mean spherical constraint cannot be met unless Λ is within $O(1/N)$ of βJ , where $2J$ is the largest eigenvalue of \mathbf{J} . If we assume the system is in the spin glass phase and write $\Lambda = \beta J + 1/2NQ(T)$ the spherical constraint equation takes the form

$$N = NQ(T) + \sum_{\lambda \neq J} \frac{1}{\beta[J - \lambda]} = NQ(T) + \frac{kTN}{J}. \quad (4)$$

In the second term on the right-hand side of equation (4) we have neglected the $O(1/N)$ difference between Λ and J . The function $Q(T)$ is the expectation value $N^{-1}\langle s_0^2 \rangle$, where s_0 is the amplitude of the $\lambda = 2J$ eigenmode. It is proportional to the usual spin glass order parameter defined by $N^{-1} \sum_i m_i^2$ [1]. From equation (4) we have $Q(T) = 1 - T/T_{SG}$ where $T_{SG} = J$ is the transition temperature below which the system is a spin glass.

Now, let us consider two copies of this model. Below T_{SG} each of these two replicas will be in a condensed, or spin glass phase, with the amplitudes of the eigenfunctions of \mathbf{J} determined by the Boltzmann factor on the right-hand side of equation (3). The overlap between the spin configurations of the two systems is

$$q = \frac{1}{N} \sum_{i=1}^N s_i^1 s_i^2 = \frac{1}{N} \sum_{\lambda} s^{(\lambda)1} s^{(\lambda)2} \quad (5)$$

where the superscripts refer to the respective replicas. The distribution function of this overlap, $\tilde{P}(q)$, is given by

$$\tilde{P}(q) = \frac{\int_{-\infty}^{\infty} \exp(-i\omega q) f(\omega) d\omega}{2\pi f(0)} \quad (6)$$

where

$$f(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty}$$

$$\times \exp\left(-\frac{1}{2} \sum_{\lambda} [(s^{(\lambda)1})^2 + (s^{(\lambda)2})^2] [2\Lambda - \beta\lambda] + \frac{i\omega}{N} s^{(\lambda)1} s^{(\lambda)2}\right) \prod_{\lambda} ds^{(\lambda)}. \quad (7)$$

Utilizing the fact that the difference between the largest eigenvalue of \mathbf{J} and any other eigenvalue of that matrix will be much larger than $1/N$, we obtain

$$f(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty}$$

$$\times \exp\left(-[(s^{(0)1})^2 + (s^{(0)2})^2] \frac{1}{2NQ(T)} + \frac{i\omega}{N} s^{(0)1} s^{(0)2}\right) ds^{(0)1} ds^{(0)2}. \quad (8)$$

Integrating over the $s^{(0)}$ s in equation (10) and then over ω in equation (6), we obtain for $P(q) = \tilde{P}(q) + \tilde{P}(-q)$,

$$P(q) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-i\omega q)}{\sqrt{1 + \omega^2 Q(T)^2}} d\omega = \frac{2}{\pi Q(T)} K_0\left(\frac{q}{Q(T)}\right) \tag{9}$$

where $K_0(y)$ is a zeroth-order modified Bessel function. The distribution function $P(q)$ is, according to Parisi, directly related to his replica-symmetry-breaking $q(x)$ via the inverse relation

$$x(q) = \int_0^q P(q') dq' \tag{10}$$

or, according to our results,

$$x(q) = \frac{2}{\pi Q(T)} \int_0^q K_0\left(\frac{q'}{Q(T)}\right) dq'. \tag{11}$$

Plots of $P(q)$ and $q(x)$, the latter obtained by inverting equation (11), are shown as figures 1(a) and 1(b).

To investigate the effect of the large, $O(N)$ fluctuations on the distribution of the free energies in the mean spherical model we consider the model with a generalized spin constraint, i.e. by setting $\sum s_i^2 = \rho N$. The quantity ρ , which is unity in the conventional normalization, is variable and corresponds, in the Bose gas picture, to the particle density.

The free energy per spin for $T < T_{SG}$ is

$$f(\rho, T) = -\rho J - \frac{T}{2} \left[-\frac{1}{2} + \ln\left(\frac{2\pi T}{J}\right) \right] \tag{12}$$

where $f(\rho, T)$ is the free energy computed for the canonical ensemble corresponding to fixed ρ . The grand canonical, or mean spherical constraint, ensemble and the canonical, or strict constraint, ensemble are related by the following integral transform in the thermodynamic limit:

$$f^g(\rho, T) = \int_{-\infty}^{\infty} \nu(x, \rho) f(x, T) dx \tag{13}$$

where $\nu(x, \rho)$ is known, in the case of the ideal Bose gas, as the Kac density [8, 9]. In the infinite volume limit, f^g is the free energy in the grand canonical, or mean constraint, ensemble. As indicated by equation (13), this free energy is given by the weighted sum over the free energies in canonical ensembles. The statistical weight of a given ensemble of the latter type, $Z_N(x, T)$, is

$$\nu(x, \rho) = \lim_{N \rightarrow \infty} \frac{N \exp(-N\Lambda x) Z_N(x, T)}{Z^{gr}(\rho, \Lambda, T)} \tag{14}$$

where the spins in Z_N satisfy $\sum_{i=1}^N s_i^2 = xN$, and the Lagrange multiplier Λ (in both numerator and denominator) is chosen to satisfy the mean constraint $\sum_{i=1}^N \langle s_i^2 \rangle = \rho N$.

It is evident that in order for the free energies f^g and f to be the same the Kac

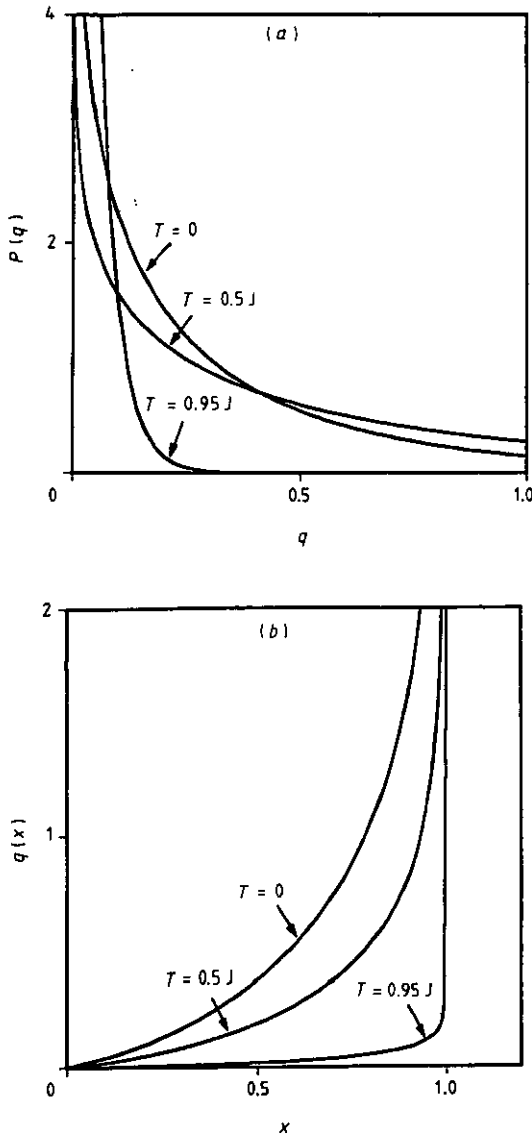


Figure 1. (a) The overlap probability distribution function, $P(q)$, for three different temperatures. (b) $q(x)$ obtained by inverting equation (11) of the text for the three cases in part (a).

density must be a delta function. However, this is not so in the condensed phase of either the spin or particle system, as we show below. For $T < T_{SG}$, $\nu(x, \rho)$ has, instead, a most interesting form.

To calculate $\nu(x, \rho)$ we first find its Fourier transform, the so-called characteristic function:

$$\lim_{N \rightarrow \infty} \left\langle \exp \left(\frac{i\xi}{N} \sum_{i=1}^N s_i^2 \right) \right\rangle = \int_0^\infty \nu(x, \rho) \exp(i\xi x) dx. \quad (15)$$

The quantity on the left-hand side represents a thermal average taken with respect to the grand canonical ensemble satisfying the mean constraint equation. One finds

$$\begin{aligned} \lim_{N \rightarrow \infty} \left\langle \exp \left(\frac{i\xi}{N} \sum_{i=1}^N s_i^2 \right) \right\rangle &= \exp(i\xi\rho) \quad (T > T_{SG}) \\ &= \sqrt{\frac{(2Q(\rho, T))^{-1}}{(2Q(\rho, T))^{-1} - i\xi}} \exp[i\xi(\rho - Q(\rho, T))] \quad (T < T_{SG}). \end{aligned} \tag{16}$$

Inverting equation (15),

$$\begin{aligned} \nu(x, \rho) &= \delta(x - \rho) \quad (T > T_{SG}) \\ &= \frac{1}{\sqrt{2\pi JQ(T)}} \frac{1}{\sqrt{x - x_c}} \exp\left(-\frac{1}{2JQ(\rho, T)}(x - x_c)\right) \Theta(x - x_c) \\ &\quad (T < T_{SG}). \end{aligned} \tag{17}$$

In the above equation $x_c = \rho - Q(\rho, T)$ and $Q(\rho, T) = \rho(1 - T/T_{SG}(\rho))$. If the above form for the Kac density is substituted into equation (13) then $f^{\#}$ can be shown to be identical to equation (12). If we now interpret equation (13) as the following average over free energies

$$f^{\#} = \int f \mathcal{D}(f) \, df \tag{18}$$

changing variables in equation (17), using equation (12), we find that the distribution function is given by

$$\mathcal{D}(f) = \frac{1}{\sqrt{2\pi JQ(T)}} \frac{1}{\sqrt{\tilde{f} - f}} \exp\left(\frac{1}{2JQ(T)}(f - \tilde{f})\right) \Theta(\tilde{f} - f) \tag{19}$$

where $\tilde{f} = [-T - (T/2)(\ln(2\pi T/J) - \frac{1}{2})]$. This expression is obtained by setting $\rho = 1$, upon doing which we recover the spherical model. The distribution for the grand canonical free energy, $f^{\#}(T)$, in equation (19) is reminiscent of the distribution for free energies conjectured by Mézard *et al* [12]. However, it differs in that it allows for extensive fluctuations in the free energy, whereas in the generalized random energy model the distribution is postulated to govern fluctuations in the free energy of order unity.

The result in equation (19) for $\mathcal{D}(f)$, and the distribution, $P(Q)$, of values of Q can both be deduced from knowledge of the Kac density, equation (17). This quantity contains the information needed to compute statistical mechanical averages in the grand canonical ensemble. The results for the spin glass order parameter and distribution of energies are surprisingly similar to the conjectures made for the Ising spin glass. At the very least, we feel that a deeper and more comprehensive study of the spherical model is called for. It would be useful, for example, to see how the results reported here can be obtained in the context of a replica-based calculation. If one can, indeed, start with a broken-replica-symmetry order parameter in the absence of replica-symmetry-breaking terms in the Hamiltonian it may be possible to treat such terms as a perturbation.

While the mean spherical model admits an order parameter function similar in form to that of Parisi [10, 11] and that obtained in simulations by Young [14] there

is an important difference. The overlaps of states taken three at a time do not possess the property of ultrametricity—a property intrinsic to the construction of $Q(x)$ due to Parisi, and assumed, as well, by Mézard *et al* [12]. Furthermore, our free energy distribution, equation (19), is missing a crucial feature of the distribution of Mézard *et al* [12]. They assume an ensemble of independently distributed free energies, whereas the distribution obtained here controls only one free energy. Finally, the properties of the spherical model spin glass reported on here are shared by spherical models with *non-random* interactions. They are not specific to a random magnetic system. All this should be taken as a caution. We nevertheless anticipate that further study of the spherical model will lead to substantial improvement of our state of knowledge regarding the microscopic structure of the spin glass phase.

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