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LETTER TO THE EDITOR

# On the thermodynamics of the spin-glass state in infinite dimension

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**Abstract.** Some exact results for the infinitely long-range Ising spin glass are derived at arbitrary temperature and magnetic field below the transition line within Parisi's replica symmetry breaking theory. The distribution of overlaps between pure states, $P(q)$, proves to be non-analytic at $q=0$ in zero field. The usual relation $S=-\partial F/\partial T$ is found to break down, showing that the thermodynamic limit and the temperature derivative do not commute in the ordered phase, at least in non-zero magnetic field. The upper breakpoint of the order parameter function and the Edwards–Anderson order parameter are rigorously derived in the low-temperature limit. The coefficient of the leading low-temperature correction to the latter turns out to be different from that derived from the TAP equations, indicating that Parisi's theory and the TAP equations may not be strictly equivalent.

The calculation of perturbational corrections to a Gaussian theory is the standard way to investigate short-range models in high but finite dimensions. In the case of spin glasses, however, up to now not too much progress has taken place in that direction. In spite of the fact that a lot of knowledge about the infinitely long-range spin glass has accumulated in the last decade (see Binder and Young 1986 and Mézard *et al* 1987 for a review), there are still serious complications which hamper progress towards a well defined field theory of the ordered phase. Understanding the physical meaning of zero modes and the spectrum of correlation lengths, as well as the nature of the marginal stability of pure states, seems to be necessary before turning to a detailed perturbational analysis. This, however, requires studies of the spin-glass phase not only in the immediate vicinity of the transition line, which was the case in most of the works in this field. In this letter some basic thermodynamic properties and the order parameter function of the infinitely long-range (Sherrington–Kirkpatrick or SK) model are studied for arbitrary temperature below $T_c$ and magnetic field less than the AT value, while other topics, such as the specific heat, Gaussian correlation lengths etc are left for future publications.

The SK model is defined for Ising spins $s_i=\pm1$ by the Hamiltonian

$$H=-\sum_{(ij)} J_{ij}s_iS_j-h\sum_{i=1}^{N} S_i$$

where $(ij)$ stands for all pairs of spins and the $J_{ij}$ are quenched independent Gaussian random exchanges with zero mean and variance $J^2/N$. The method of Mézard and Virasoro (1985) will be used to calculate, within Parisi's scheme, thermodynamic functions such as the free energy

$$F=-kT\,\overline{\log Z} \tag{1a}$$

energy

$$E=-\overline{\sum_{(ij)} J_{(ij)}\langle S_i s_j\rangle} \qquad (1b)$$

magnetisation

$$M=\overline{\sum_{i=1}^{N}\langle S_i\rangle} \qquad (1c)$$

and entropy

$$S=\frac{1}{T}(E-F-Mh) \qquad (1d)$$

where $Z=\operatorname{Tr}\exp(-H/kT)$, $\langle\ldots\rangle$ and $\overline{\ldots}$ stand for the full thermodynamic and bond configurational averages, respectively. Units will be chosen chosen so that $J=k=1$. In terms of Parisi's order parameter function $q(x)$, the following formulae for the stable stationary point can be derived (see also Parisi 1980, Duplantier 1981, de Almeida and Lage 1983, Goltsev 1984, Sommers and Dupont 1984 and Binder and Young 1986):

$$\frac{1}{N}F=\frac{1}{4T}\left(2q_1-1-\int_0^1 \mathrm{d}x q(x)^2\right)-T\int_{-\infty}^{\infty}\frac{\mathrm{d}y}{\sqrt{2\pi}}\mathrm{e}-y^2/2g(x_0,\sqrt{q_0}y+h) \qquad (2a)$$

$$\frac{1}{N}E=\frac{1}{2T}\left(\int_0^1 \mathrm{d}x q(x)^2-1\right) \qquad (2b)$$

$$\frac{1}{N}M=\int_{-\infty}^{\infty}\frac{\mathrm{d}y}{\sqrt{2\pi}}\mathrm{e}-y^2/2m(x_0,\sqrt{q_0}y+h) \qquad (2c)$$

where $x_0$ is the breakpoint of $q(x)$ corresponding to the minimal value of overlaps $q_0$, while $q_1$ is the Edwards-Anderson order parameter, i.e. the maximum of $q(x)$. The auxiliary functions $g(x,y)$ and $m(x,y)$ satisfy the equations (de Almeida and Lage 1983, Goltsev 1984, Sommers and Dupont 1984 and Mézard and Virasoro 1985):

$$\frac{\partial m}{\partial x}+\tfrac{1}{2}q'(x)\frac{\partial^2 m}{\partial y^2}=-\frac{1}{2T}xq'(x)\frac{\partial(m^2)}{\partial y} \qquad \text{with } m(x_1,y)=\tanh\frac{y}{T} \qquad (3a)$$

$$\frac{\partial g}{\partial y}=\frac{1}{T}m \qquad (3b)$$

($x_1$ corresponds to $q_1=q(x_1)$). In order to determine $q(x)$, we must use the stationary condition (Mézard and Virasoro 1985):

$$q(x)=\int_{-\infty}^{\infty}\mathrm{d}yN(x,y)m(x,y)^2 \qquad (4a)$$

where $N(x,y)$ obeys the equation

$$\frac{\partial N}{\partial x}-\tfrac{1}{2}q'(x)\frac{\partial^2 N}{\partial y^2}=-\frac{1}{T}xq'(x)\frac{\partial(Nm)}{\partial y} \qquad \text{with } N(x_0,y)=\frac{1}{\sqrt{2\pi q_0}}\exp\left(-\frac{(y-h)^2}{2q_0}\right) \qquad (5)$$

A clear intepretation of the functions $N$ and $m$ in terms of a hierarchical organisation of clusters of lattice sites was given by Mézard and Virasoro (1985), although they did not write down equation (5) explicitly (see, however, Sommers and Dupont (1984), where this equation has appeared, but with a different and somewhat problematic interpretation of $N(x, y)$ as a distribution of internal frozen fields).

Differentiating ($4a$) with respect to $x$, using ($3a$), (5) and integrating by parts, we can derive a set of additional equations (Sommers and Dupont 1984):

$$1=\int_{-\infty}^{\infty} \mathrm{d}y N(x,y)\left(\frac{\partial m(x,y)}{\partial y}\right)^2 \tag{4b}$$

$$\frac{2}{T}x\int_{-\infty}^{\infty} \mathrm{d}y\, N(x,y)\left(\frac{\partial m(x,y)}{\partial y}\right)^3=\int_{-\infty}^{\infty} \mathrm{d}y\, N(x,y)\left(\frac{\partial^2 m(x,y)}{\partial y^2}\right)^2 \tag{4c}$$

etc. Instead of considering ($4a$) for arbitrary $x$, we will use equations ($4a, b, \ldots$) at the value $x_0$, thus exploiting the fact that $N(x_0, y)$ is a simple Gaussian. The solution is sought in the form of the following ansatz:

$$m(x,y)=(A_0+A_1x+\ldots)y+(B_0+B_1x+\ldots)y^3+\ldots \tag{5a}$$

$$q(x)=ax+bx^2+cx^3+dx^4+\ldots \tag{5b}$$

$$h^2=\tilde{a}x_0^3+\tilde{b}x_0^4+\tilde{c}x_0^5+\ldots \tag{5c}$$

where the coefficients are functions of $T$. Comparing terms order by order, it turns out that all the coefficients can be expressed by means of the $A_i$, furthermore $A_0\equiv 1$. It can be proved that $A_0$ is actually the zero-field susceptibility, which is constant below $T_c$ (Sompolinsky 1981, Goltsev 1984). Now, taking into account the initial condition of ($3a$), an infinite system of algebraic equations remains for the $A_i$ ($i = 1, 2, \ldots$) and $x_1$, which can be solved for arbitrary temperature, at least in principle, by truncation.

The results obtained from the above scheme can be summarised as follows.

(i) $q(x)$ and $x_1$ (and hence the Edwards-Anderson order parameter $q_1$ itself) depend only on temperature. This is in fact one, and the only one, of the set of statements known as the Parisi-Toulouse hypothesis (Parisi and Toulouse 1980, Vannimenus *et al* 1981) which thus proved to be rigorously true.

(ii) We find for the expansion coefficients of the order parameter function

$$\begin{aligned} &a=2TA_1^2 \qquad b=0\\ &c=\tfrac{2}{3}T(21A_1^4-16A_1^2A_2-8A_2^2) \qquad d=-32TA_1^5 \qquad \ldots . \end{aligned} \tag{6}$$

The non-vanishing of $d$ is rather surprising, because it means that the probability distribution of overlaps between pure states, $P(q)=x(q)'$ (Parisi 1983), does have odd powers in its series around $q=0$. Since $P(q)$ is an even function due to the spin-inversion symmetry in zero magnetic field, it must therefore be non-analytic at zero overlap.

(iii) The dependence of $x_0$ on the magnetic field, ($5c$), is closely related to $q(x)$:

$$\tilde{a}=\frac{2}{3T}a^2 \qquad \tilde{b}=0 \qquad \tilde{c}=\frac{1}{5T}a\left(\frac{3}{T}a^2+8c\right) \qquad \ldots . \tag{7}$$

(iv) We find for the magnetic field dependence of thermodynamic functions at arbitrary temperature (denoting by $\Delta$ the deviation from the zero-field value):

$$\Delta\frac{F}{N}=-\tfrac{1}{2}h^2+\tfrac{3}{20}(\tfrac{3}{2})^{2/3}(aT)^{-1/3}h^{10/3}+\dots \tag{8a}$$

$$\Delta\frac{E}{N}=\tfrac{1}{2}h^2-\tfrac{9}{20}(\tfrac{3}{2})^{2/3}(aT)^{-1/3}h^{10/3}+\dots \tag{8b}$$

$$\Delta\frac{M}{N}=h-\tfrac{1}{2}(\tfrac{3}{2})^{2/3}(aT)^{-1/3}h^{7/3}+\dots \tag{8c}$$

$$\Delta\frac{S}{N}=-\frac{1}{10T}(\tfrac{3}{2})^{2/3}(aT)^{-1/3}h^{10/3}+\dots. \tag{8d}$$

Near $T_c=1$, where $a\simeq\frac{1}{2}$, equation (8$c$) agrees with the result of Parisi and Toulouse (1980), while (8$c$) and (8$d$) prove that the projection hypothesis of Parisi and Toulouse (1980) and Vannimenus *et al* (1981) for the entropy and magnetisation is not rigorously exact (this has also been noted by Elderfield (1983)).

The usual relationship between entropy and free energy, $-S=\partial F/\partial T$, seems to be a good check on the above formulae. In order for it to be satisfied, $a(T)$ should be the solution of the following differential equation:

$$\frac{d}{dT}(aT)^{-1/3}=\frac{2}{3T}(aT)^{-1/3}$$

which would imply $a(T)\sim T^{-3}$. An extended series expansion near $T_c$, to be published in a subsequent paper, however, excludes this possibility. Furthermore, it is not consistent with the reasonable expectation $a\sim T^{-1}$ for the low-temperature behaviour (Vannimenus *et al* 1981). The above anomaly can be understood as follows: the order of thermodynamic limit and temperature derivative cannot be interchanged in the replica symmetry breaking phase, at least in a non-zero magnetic field, i.e. subdominant terms in the free energy are extremely fast-varying functions of temperature for $N\to\infty$. A similar behaviour in the case of energy and magnetisation can also be predicted. This observation is reminiscent of other features of the spin-glass state, such as the lack of self-averaging and reproducibility, and it is presumably connected to the multi-valley structure of phase space.

Finally, we present some exact results in the low-temperature limit. For $x=x_1$, equations (4$a$)-4$c$) take the form

$$q_1-1=\int_{-\infty}^{\infty}dy\,N(x_1,y)\left(\tanh^2\frac{y}{T}-1\right)\qquad T^2=\int_{-\infty}^{\infty}dy\,N(x_{1,y})\cosh^{-4}\frac{y}{T}$$

$$x_1\int_{-\infty}^{\infty}dy\,N(x_{1,y})\cosh^{-6}\frac{y}{T}=2\int_{-\infty}^{\infty}dy\,N(x_{1,y})\tanh^2\frac{y}{T}\cosh^{-4}\frac{y}{T}.$$

For $T\to 0$, only the range around zero contributes in leading order, yielding:

$$q_1=1-\tfrac{3}{2}T^2+\dots \tag{9a}$$

$$x_1=\tfrac{1}{2}+\dots \tag{9b}$$

$$N(x_1,0)=\tfrac{3}{4}T+\dots. \tag{9c}$$

Equation (9$a$) has been found by Parisi and Toulouse (1980) along the AT line and it was extended to arbitrary magnetic field below the transition line by their projection hypothesis. The new ingredient here is that $q_1$ is *proved* to be independent of magnetic field. Hence the factor $\frac{3}{2}$ is exact and can be compared with the value 1.810 found by Bray and Moore (1979) using the TAP theory and an assumption about the existence of a zero mode. Considering that this latter actually proved to be true (Goltsev 1984, Kondor and De Dominicis 1986), this discrepancy is a signal that the two theories of the long-range spin glass, the replica symmetry breaking scheme of Parisi and the TAP equations, are not equivalent. The exact limiting value of $x_1$ found here, $\lim_{T\to 0} x_1 = \frac{1}{2}$, can be deduced also from a scaling assumption $q(x) = f(x/T)$, where $f$ is a scaling function (Vannimenus *et al* 1981). This simple form of the order parameter function, however, cannot be extended to temperatures far away from zero, as can be seen by expanding $q(x)$ near $T_c$. Details of this will be given in a subsequent publication.

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