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A new simple version of the replica method

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Abstract. The moments of the partition function of a disordered system are used to determine the probability distribution of the free energy. The relation between them is essentially given by a Legendre transformation. A cut-off must be introduced to ensure the normalization of the distribution function. The method yields reasonable approximations or even rigorous results for the mean free energy without taking into account replica symmetry breaking (RSB). It therefore represents a conceptually and technically simple alternative to Parisi's RSB-scheme. Investigated examples are the random-energy model and the Sherrington–Kirkpatrick model of spin glasses.

1. Introduction

The replica trick is a tool which is often used to calculate the mean free energy and further interesting quantities of disordered systems [1, 2]. The starting point is the observation that it is usually much easier to evaluate moments $\langle Z^n \rangle = \exp \Phi(n)$ of the partition function Z than the averaged logarithm of Z determining the free energy F of the system $\langle \ln Z \rangle = -\beta \langle F \rangle$. (Here the brackets denote the average over the randomness of the system.) The basic idea of the conventional replica trick is to obtain the mean free energy by performing the limit

$$\langle \ln Z \rangle = \lim_{n \to 0} \frac{\langle Z^n \rangle - 1}{n} = \left. \frac{\mathrm{d}\Phi}{\mathrm{d}n} \right|_{n=0}. \tag{1}$$

The problematic aspect of the procedure resides in the fact that in most interesting cases the function $\Phi(n)$, originally calculated for integer values of n, shows a second-order phase transition or even a sequence of phase transitions in the interval $0 < n < 1$ and that, therefore, a simple continuation of $\Phi(n)$ from natural integers to $n = 0$ leads to erroneous results. These phase transitions are associated with the so-called replica symmetry breaking (RSB). Parisi [3, 4] invented a scheme to take into account RSB and, in the case of the Sherrington–Kirkpatrick (SK) model of spin glasses [2, 5], he was able to construct a valid continuation of the function $\Phi(n)$ towards the limit $n = 0$. The method has been applied with success to a lot of models [11] and is generally believed to be correct. However, the computational effort demanded by this procedure is sometimes considerable and the interpretation of the involved quantities, even if possible and instructive, is not always simple. Moreover, there are interesting cases for which it is unclear how to apply Parisi's scheme.

This paper proposes a simple alternative concept to circumvent the difficulties outlined above. The basic idea is now that, instead of performing the transition to $n = 0$ in the function $\Phi(n)$, one could try to construct the distribution function for the free energy directly from the function $\Phi(n)$. It turns out that, in order to do this, it is not necessary to know the function $\Phi(n)$ in the whole range of n, but only above a certain threshold value n_0 and that therefore

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reasonable approximations and sometimes even rigorous results can be found without taking into account RSB which is important only in the vicinity of $n = 0$.

In section 2 the general formulae of the method are developed. In order to demonstrate the efficiency and also the limits of the proposed scheme, applications to two well-investigated examples, the random-energy model (REM) [6, 7] and the SK model of spin glasses [2, 5], are presented in sections 3 and 4, respectively.

2. Basic equations

Let us suppose the function $\langle Z^n \rangle = \exp \Phi(n)$ to be known within a certain range of n. We are interested in the distribution function of the free energy F. Instead of F we shall use the dimensionless quantity $Y = -\beta F = \ln Z$. Its distribution function will be denoted by $w(Y) = \exp(-R(Y))$. The relation between the functions Φ and R is given by

$$\langle Z^n \rangle = \mathrm{e}^{\Phi(n)} = \int \mathrm{d}Y \, w(Y) \mathrm{e}^{nY} = \int \mathrm{d}Y \, \mathrm{e}^{(nY - R(Y))}. \tag{2}$$

In order to derive $R(Y)$ from $\Phi(n)$, let us further assume that the integrand in equation (2) shows a well-pronounced maximum and that the integral can be evaluated by means of the saddle-point approximation. The maximum of the exponent

$$\frac{\mathrm{d}}{\mathrm{d}Y}(nY - R(Y)) = 0 \Rightarrow \frac{\mathrm{d}R}{\mathrm{d}Y} = n \tag{3}$$

defines a function $Y(n)$. Expansion of the exponent around this point leads to

$$\Phi(n) = \left[nY - R(Y) - \frac{1}{2} \ln \frac{1}{2\pi} \frac{\mathrm{d}^2 R}{\mathrm{d}Y^2} \right]_{Y(n)}. \tag{4}$$

Using equation (3) and differentiating with respect to n yields

$$\Phi(n) = nY - R(Y) + \tfrac{1}{2} \ln 2\pi Y' \tag{5}$$

$$\Phi'(n) = Y + \frac{1}{2} \frac{Y''}{Y'} \tag{6}$$

where all Y have to be understood as $Y(n)$ and the primes denote derivatives with respect to n.

Combining equations (3), (5) and (6) we find the following transformation between $\Phi(n)$ and $R(Y)$

$$Y - \frac{\mathrm{d}\Phi}{\mathrm{d}n} = -\frac{1}{2} \frac{Y''}{Y'} \tag{7a}$$

$$R - n \frac{\mathrm{d}\Phi}{\mathrm{d}n} + \Phi = \frac{1}{2} \ln 2\pi Y' - \frac{n}{2} \frac{Y''}{Y'} \tag{7b}$$

$$\frac{\mathrm{d}R}{\mathrm{d}Y} - n = 0. \tag{7c}$$

The left-hand sides of equations (7) represent the well known Legendre transformation. In reasonable models Y and Φ have to be extensive quantities. It follows that the same must hold for R. Thus, in the thermodynamic limit, the transition from $\Phi(n)$ to $R(Y)$ is simply given by the Legendre transformation. The terms on the right-hand side of equations (7) represent finite-size corrections. The Legendre transformation (7) without finite-size corrections has already been derived in [13].

The situation is sketched schematically in figure 1. The value of $\Phi(n)$ is mainly determined by the distribution of Y in the neighbourhood of $Y(n)$. Higher values of n belong to higher values of Y. Thus, the function $\Phi(n)$ in the range $n \geqslant 1$ provides only information about

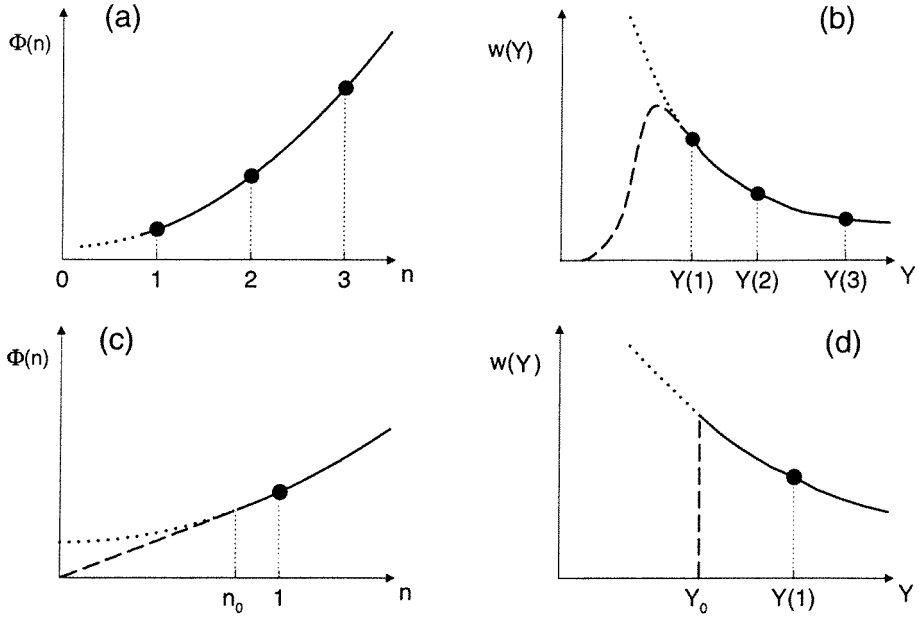

Figure 1. Legendre transformation between $\Phi(n)$ and $w(Y)$ (schematically). Dotted curves represent simple analytic continuations. Dashed lines in (*c*) and (*d*) indicate the cut-off and the corresponding tangent on $\Phi(n)$.

the tail of the distribution function. We are mainly interested in the maximum region. At first glance it might seem impossible to infer the shape of the distribution function near the maximum from its tail. Indeed, a simple extrapolation of the tail would lead to a similar failure as the simple analytic continuation of $\Phi(n)$ towards $n = 0$ (dotted curves in figure 1). The turn down of $w(Y)$ in the maximum region corresponds to the phase transition in $\Phi(n)$.

However, there is a simple requirement fixing the position of this transition to some extent. That is the normalization of the distribution. Therefore, the crudest approximation for $R(Y)$ can be obtained by carrying out the transformation prescribed by equations (7) and then introducing a lower cut-off at some Y_0 according to the normalization condition

$$\int_{Y_0}^{\infty} \mathrm{d}Y\, \mathrm{e}^{-R(Y)} = 1. \tag{8}$$

An expansion of $R(Y)$ at Y_0 approximately yields

$$R(Y_0) + \ln R'(Y_0) = R(n_0) + \ln n_0 = 0 \tag{9}$$

with $Y_0 = Y(n_0)$ and $R(Y(n_0)) = R(n_0)$. In the thermodynamic limit this condition reduces to $R(n_0) = 0$. The logarithmic term again provides a finite-size correction. For the mean free energy one obtains

$$\langle Y \rangle = \int_{Y_0}^{\infty} \mathrm{d}Y\, Y \mathrm{e}^{-R(Y)} \approx Y_0 \tag{10}$$

plus finite-size corrections which are not well determined at this stage because of the rather crude approximation of the cut-off and therefore will be neglected in the following. Refinements are possible and will be discussed elsewhere. With the aid of equation (7*b*), the cut-off in the distribution function can be translated into a modification of $\Phi(n)$ for small $n \leqslant n_0$. In the thermodynamic limit the result is simply a replacement of $\Phi(n)$ by a tangent

passing through the origin and joining the original curve at $n = n_0$ (see figures 1(c) and (d)). The slope of the tangent $\Phi'(n_0)$ represents the mean free energy in agreement with equations (7a) and (10). A remark made by Kondor [8] indicates that analogous constructions have already been used by Derrida and Rammal in order to estimate the free energies of the REM and SK models, respectively.

Provided the exact $\Phi(n)$ is used, the procedure described above leads back to the conventional replica trick (1). Indeed, the exact function $\Phi(n)$ must obey the condition $\Phi(0) = 0$ and the requirement of convexity $\mathrm{d}^2\Phi/\mathrm{d}n^2 \geqslant 0$ [9]. Both properties together signify that the tangent touches the curve at the point $n_0 = 0$ and that, consequently, the slope of the tangent becomes $\langle Y \rangle = \Phi'(n_0) = \Phi'(0)$.

The expansions contained in equations (4) and (9) are allowed under the conditions

$$|Y''| \ll |Y'|^{\frac{3}{2}} \tag{11a}$$

$$\frac{1}{n_0^2} \ll |Y'|. \tag{11b}$$

An iterative evaluation of Y from equation (7a) is possible if the condition

$$|Y''| \ll |Y||Y'| \tag{11c}$$

is fulfilled. Y being an extensive quantity, all these conditions are usually satisfied in the thermodynamic limit as long as the derivatives do exist. In finite systems they have to be checked.

3. Random-energy model

As a first example we shall consider the REM introduced by Derrida [6]. It is defined by the following properties: The system has $M = 2^N$ energy levels E_k which are independent random variables with Gaussian distribution. In the simplest version all mean values are put to zero, $\langle E_k \rangle = 0$, and the variances are chosen as $\langle E_k^2 \rangle = N/2$.

Derrida found exact solutions of this model in the thermodynamic limit $N \to \infty$ and also gave finite-size corrections. The usual replica trick does not lead to reasonable results as long as replica symmetric expressions are used. Later on Gross and Mézard [7] showed that the correct results can be obtained by means of Parisi's scheme of RSB. In the following we derive the correct results applying the procedure developed in section 2 to replica symmetric estimates of the moments $\langle Z^n \rangle$.

In the case of low temperatures the partition function is dominated by the lowest energy level corresponding to the ground state of the system. Then the moments can be approximated by

$$\mathrm{e}^{\Phi(n)} = \langle Z^n \rangle = \left\langle \sum_{k_1 \ldots k_n = 1}^{M} \mathrm{e}^{-\beta(E_{k_1} + \cdots + E_{k_n})} \right\rangle \approx \sum_k \langle \mathrm{e}^{-n\beta E_k} \rangle \tag{12}$$

because all replicas occupy the same ground state $k_1 = k_2 = \cdots = k_n = k$. The result for $\Phi(n)$ is

$$\Phi(n) = \frac{n^2\beta^2}{2} \langle E_k^2 \rangle + \ln M = N \left(\frac{n^2\beta^2}{4} + \ln 2 \right). \tag{13}$$

Obviously this approximation breaks down in the limit $n \to 0$ because of $\Phi(0) \neq 0$.

Transformation (7) yields

$$\begin{aligned} Y &= \frac{\mathrm{d}\Phi}{\mathrm{d}n} = Nn\frac{\beta^2}{2} \qquad Y'' = 0 \\ R &= n\frac{\mathrm{d}\Phi}{\mathrm{d}n} - \Phi + \frac{1}{2}\ln 2\pi Y' = N\left[\frac{n^2\beta^2}{4} - \ln 2\right] + \frac{1}{2}\ln \pi\beta^2 N. \end{aligned} \tag{14}$$

The cut-off condition (9) takes the form

$$n_0 = \frac{2}{\beta}\sqrt{\alpha} \qquad \alpha = \ln 2 - \frac{1}{2N}\ln 4\pi\alpha N \tag{15}$$

and for the mean free energy we obtain

$$Y_0 = Y(n_0) = N\beta\sqrt{\alpha} \qquad \langle F\rangle \approx -kTY_0 = -N\sqrt{\alpha}. \tag{16}$$

This free energy is temperature independent. The system is frozen in.

In the opposite limit of high temperatures the approximation

$$\begin{aligned} &\langle Z^n\rangle \approx \langle Z\rangle^n \\ &\Phi(n) \approx n\Phi(1) = nN\left(\frac{\beta^2}{4} + \ln 2\right) \end{aligned} \tag{17}$$

can be used. Transformation (7) leads to

$$\begin{aligned} Y &= N\left(\frac{\beta^2}{4} + \ln 2\right) = Y_0 \approx -\beta\langle F\rangle \\ \langle F\rangle &= -N\left(\frac{\beta}{4} + \frac{1}{\beta}\ln 2\right). \end{aligned} \tag{18}$$

In this approximation Y does not depend on n. This means that fluctuations of the free energy are not taken into account at all. The distribution function of Y reduces to a δ-like function.

In the thermodynamic limit $N \to \infty$ the results (15), (16) and (18) are exact. The phase transition between the low-temperature phase (16) and the high-temperature phase (18) takes place at $\beta_c = 2\sqrt{\ln 2}$.

In finite systems equation (15) provides logarithmic corrections to the energy of the low-temperature phase which are also in agreement with the results given by Derrida [6]. In this case the phase transition is smeared out. Hence the low- and high-temperature results do not completely fit together. In figure 2 computer simulations for a rather small system with $M = 100$ states ($N = 6.644$) are compared with the analytic estimates (15), (16) and (18). Good agreement for high and low temperatures and deviations in the neighbourhood of the transition temperature are observed. The variances of the free energy are plotted in figure 3. In the limit $T \to 0$ the computer simulations agree well with the results obtained from the low temperature approximation (equations (14), (15)) of the distribution function.

In his original paper Derrida also considered generalizations of the REM by including an 'external field' as well as 'ferromagnetic interactions'. These extensions lead to more complex phase diagrams. In these cases, too, the exact results obtained by Derrida can be completely reproduced in the way outlined above for the basic model.

4. SK model

One of the most investigated spin glass models is that of Sherrington and Kirkpatrick [2, 5]. It was just this model which led to the discovery of RSB [10] and gave rise to Parisi's invention of a scheme to treat this phenomenon [3, 4]. It is therefore tempting to apply the proposed method

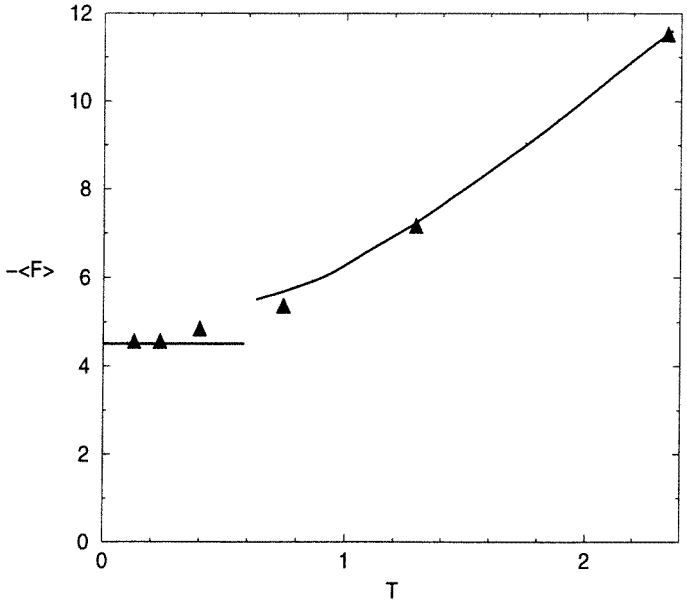

Figure 2. Free energy of a finite REM with $M = 100$ states. Full lines represent the low- and high-temperature approximations. The points are results of a computer simulation.

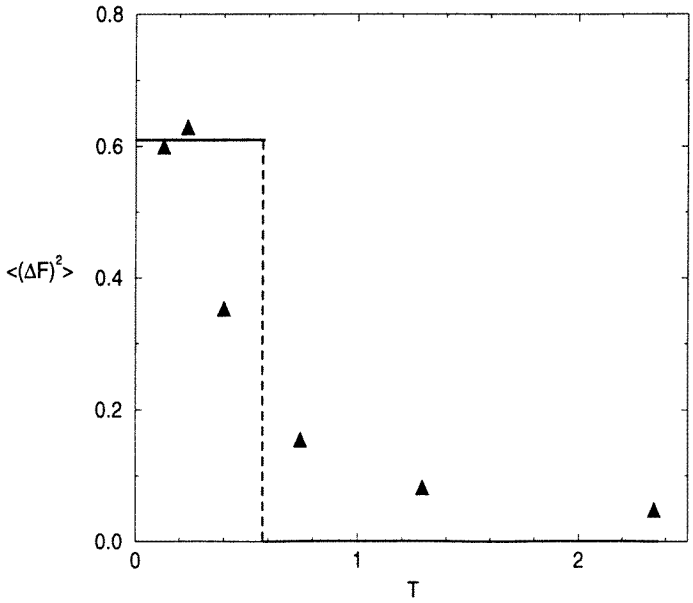

Figure 3. Variances of the free energy for the REM of figure 2.

to this model in order to test its reliability. We shall use the replica-symmetric approximations for the moments given already by Kirkpatrick and Sherrington [2] which are valid for higher values of n but are known to fail in the limit $n \to 0$.

The model consists of N Ising spins. Each pair of spins, independently of their distance,

interacts via a coupling constant J_{ij}. These parameters are independent random variables obeying a Gaussian distribution with vanishing mean value $\langle J_{ij}\rangle = 0$ and variance $\langle J_{ij}^2\rangle = 1/N$. The replica-symmetric estimate for the moments calculated in [2] has the form

$$\begin{aligned}
&\Phi(n) = NA(n, q, \beta)\\
&A(n, q, \beta) = \frac{\beta^2}{4}[n(1-q)^2 - n^2q^2] + n\ln 2 + \ln I_n(\beta\sqrt{q})\\
&I_n(\gamma) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-\frac{t^2}{2}}(\cosh\gamma t)^n.
\end{aligned} \tag{19}$$

The variational parameter q is determined by minimization

$$\frac{\partial A}{\partial q} = 0 \qquad q = \frac{\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{-\frac{t^2}{2}}(\cosh\gamma t)^n(\tanh\gamma t)^2}{\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{-\frac{t^2}{2}}(\cosh\gamma t)^n} \qquad \gamma = \beta\sqrt{q}. \tag{20}$$

Inserting the solution $q(n, \beta)$ in equation (19) one obtains $\Phi(n, \beta)$. Then one can perform the Legendre transformation (7) which, in the thermodynamic limit, leads to

$$\begin{aligned}
&Y = \frac{\mathrm{d}\Phi}{\mathrm{d}n} = N\frac{\mathrm{d}A}{\mathrm{d}n} = N\left[\frac{\partial A}{\partial n} + \frac{\partial q}{\partial n}\frac{\partial A}{\partial q}\right] = N\frac{\partial A}{\partial n}\\
&R = nY - \Phi = N\left(n\frac{\partial A}{\partial n} - A\right).
\end{aligned} \tag{21}$$

Here the partial derivatives refer to $A(n, q, \beta)$ and q is replaced by $q(n, \beta)$ only after the derivation. The cut-off condition (9) takes the form

$$R(n_0) = 0 \qquad n\frac{\partial A}{\partial n}\bigg|_{n_0} = A|_{n_0}. \tag{22}$$

Having determined $n_0(\beta)$ we obtain the mean free energy according to equation (10)

$$F = -\frac{1}{\beta}Y_0 = -\frac{N}{\beta}\frac{\partial A}{\partial n}\bigg|_{n_0} = -\frac{N}{\beta}\frac{A}{n}\bigg|_{n_0}. \tag{23}$$

Differentiating F, we can derive the energy and entropy per spin

$$\begin{aligned}
&\frac{S}{N} = -\frac{1}{N}\frac{\mathrm{d}F}{\mathrm{d}T} = \frac{A}{n} - \frac{\beta}{n}\frac{\partial A}{\partial\beta} = \frac{A}{n} + \frac{\beta^2}{2}[q^2(1-n) - 1]\\
&\frac{U}{N} = \frac{1}{N\beta}(\beta F + S) = -\frac{1}{n}\frac{\partial A}{\partial\beta} = \frac{\beta}{2}[q^2(1-n) - 1]
\end{aligned} \tag{24}$$

where equations (19), (20) and (22) have been used several times to simplify the expressions and q and n_0 are determined as functions of β by equations (20) and (22).

For temperatures above the critical value 1 ($\beta \leqslant 1$) the only solution of equation (20) is $q = 0$. Then A reduces to $A = n(\beta^2/4 + \ln 2)$ and equation (22) is satisfied for all n. The solutions for the energy and entropy are

$$\frac{U}{N} = -\frac{\beta}{2} \qquad \frac{S}{N} = -\frac{\beta^2}{4} + \ln 2 \qquad (\beta \leqslant 1) \tag{25}$$

in agreement with previous results [2]. For lower temperatures equation (20) admits a non-trivial solution which can be evaluated numerically and provides the thermodynamic quantities of the spin glass phase. The resulting curves for U and S are plotted in figures 4 and 5, respectively. They only slightly differ from the results obtained by Parisi [4] in a one-step RSB procedure despite us having used only replica-symmetric approximations. On the other hand there is a considerable difference to the replica-symmetric solution obtained by Kirkpatrick and Sherrington [2] within the framework of the ordinary replica trick. However, the result

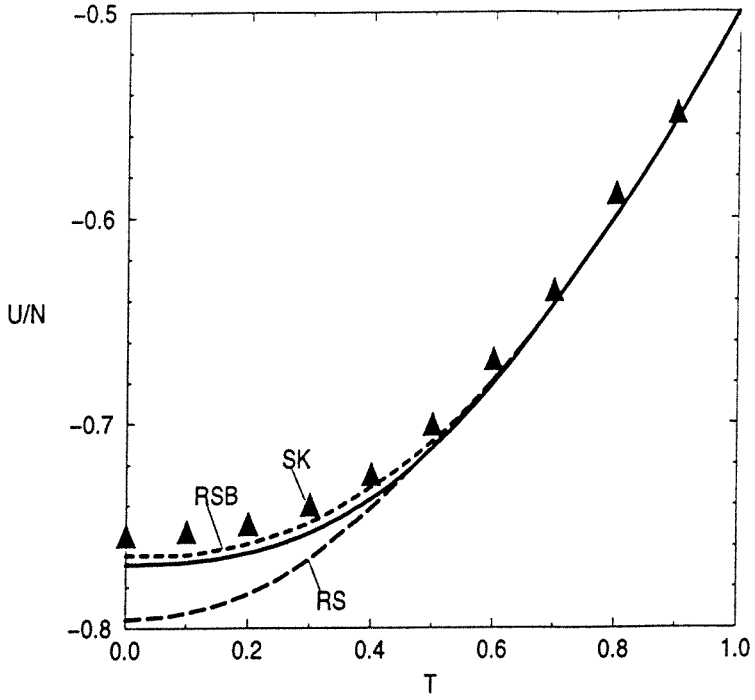

Figure 4. Energy per spin in the SK model. Full curve: present result; RS: replica-symmetric result [2]; RSB: one-step replica-symmetry breaking [4]; SK: computer simulations [2].

displayed in figure 5 also shows that our method cannot be rigorous because the entropy does not vanish in the zero-temperature limit. We find -0.03 which is clearly better than the original value -0.16 in [2] but nevertheless this demonstrates the approximative character of the method.

5. Discussion

The method considered in this paper differs from the ordinary replica method by using the idea of deriving the probability distribution of the free energy immediately from the function $\Phi(n) = \ln\langle Z^n\rangle$. It is clear that the validity of the results obtained for the free energy depends on the correctness of the approximations used for $\Phi(n)$. The advantage of the proposed procedure in comparison with the usual one relies on the fact that the limit $n \to 0$ in the function $\Phi(n)$ need not be performed. Usually it suffices to know the function $\Phi(n)$ only above a certain cut-off value n_0. Decisive in the influence of RSB is whether the critical value n_c for the inset of RSB lies above n_0 or not. Detailed investigations show that in the REM n_0 and n_c coincide whereas for the SK model n_c lies clearly above n_0 [8]. Therefore, in the REM it is possible to find the rigorous result without taking into account RSB. In contrast, in the SK model we obtain only approximate results. One has to bear in mind, however, that the phase transition is of higher order and that just below n_c the replica-symmetric solution of $\Phi(n)$ only slightly deviates from the correct RSB-result. Therefore, replica-symmetric calculations can be expected to provide reasonable approximations for the free energy also in such cases with $n_0 < n_c$.

The simple cut-off procedure used in this paper is similar to the one-step RSB and the cut-

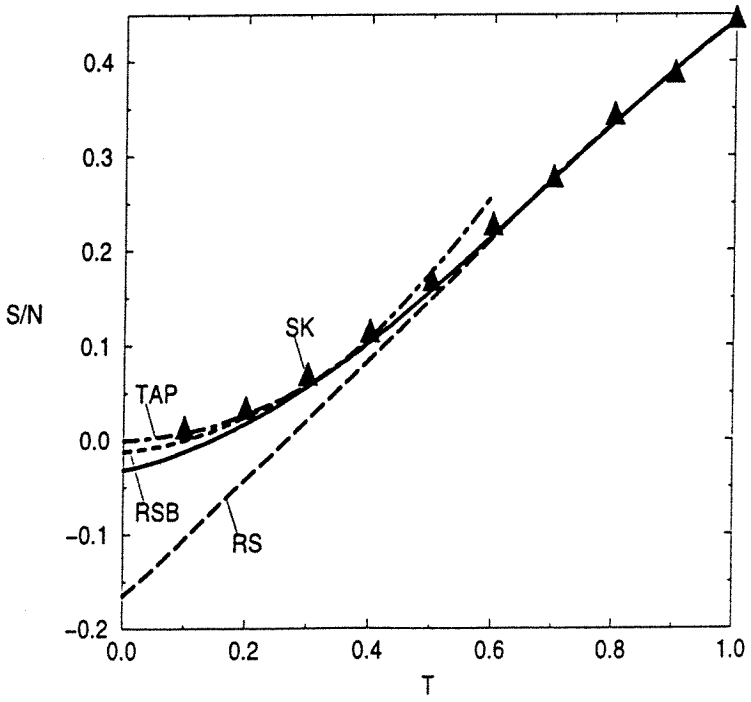

Figure 5. Entropy per spin in the SK model: notations as in figure 4. TAP: [12].

off parameter n_0 can be shown to correspond to the position of the step in the overlap spectrum $q(x)$ [4, 7]. A continuous overlap function $q(x)$ would certainly imply that the cut-off in the distribution function $w(Y)$ should be replaced by a continuous transition. At the moment we do not know how to formulate an appropriate extension of the method. Further examples will be treated in a forthcoming paper.

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