Free energy fluctuations in Ising spin glasses

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The sample-to-sample fluctuations of the free energy in finite-dimensional Ising spin glasses are calculated, using the replica method, from higher order terms in the replica number \( n \). It is shown that the Parisi symmetry breaking scheme does not give the correct answers for these higher order terms. A modified symmetry breaking scheme with the same stability is shown to resolve the problem.

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The Parisi replica symmetry breaking scheme [1, 2, 3, 4] was a milestone in the study of spin glasses. It was proposed as long ago as 1979 and has been extensively used ever since. It is the purpose of this Letter to point out that an important modification of it is needed in order to calculate the sample-to-sample fluctuations of spin glasses.

The replica method is usually used in spin glasses to calculate the average free energy \( F \) as a function of inverse temperature \( \beta \) from the partition function \( Z \) via

\[
\beta F = -\ln Z = -\lim_{n \to 0} \frac{1}{n} \ln Z^n. \tag{1}
\]

The overbar means averaging over bond configurations. Apart from the free energy, the replica method also gives in principle access to other physical quantities as well. Expanding the logarithm on the right hand side in Eq. (1) one gets

\[
\ln Z^n = -n \beta F + \frac{n^2}{2} \beta^2 \Delta F^2 + \cdots, \tag{2}
\]

where \( \Delta F^2 = \left( \ln Z - \ln Z^n \right)^2 / \beta^2 \) is the mean-square sample-to-sample fluctuation of the free energy, and the coefficients of the higher order terms are higher order cumulants. In order to obtain the coefficients in this expansion from the replica method, it is necessary to keep the replica number \( n \) small but finite throughout the calculation (as opposed to the case of the free energy itself where it is possible to set \( n = 0 \) early on), which makes it rather cumbersome. Moreover, using Parisi’s replica symmetry breaking scheme [1, 2, 3, 4, 5], it will be shown below that the coefficients so obtained differ when assuming \( n \) positive or negative. Note that the replica method intrinsically requires \( n \) to be non-integer, and that it is no more unnatural to take \( n \) negative than it is to take it non-integer. Thus conflicting answers are obtained for the same physical quantity which indicates that there is a problem with Parisi’s replica symmetry breaking scheme. We will argue that the correct answer is in fact given by the \( n < 0 \) solution. Furthermore we show how the symmetry breaking scheme can be modified to give the correct results when \( n > 0 \). However, this new replica symmetry breaking scheme gives the same results as Parisi’s scheme for quantities like the free energy or the distribution of spin overlaps \( P(q) \), and has the same stability.

We start from the usual replica field theory for \( d \)-dimensional spin glasses as derived, e.g., in [5] or [3], where we have a free energy functional

\[
\mathcal{H}_{\text{rep}}\{q_{\alpha\beta}\} = \int d^d x \left[ -\frac{\tau}{2} \sum_{\alpha,\beta} q_{\alpha\beta}^2 + \frac{1}{4} \sum_{\alpha,\beta} (\nabla q_{\alpha\beta})^2 \right. \\
\left. - \frac{w}{6} \sum_{\alpha,\beta,\gamma} q_{\alpha\beta} q_{\beta\gamma} q_{\gamma\alpha} - \frac{y}{12} \sum_{\alpha,\beta} q_{\alpha\beta}^4 \right] \tag{3}
\]

and

\[
\overline{Z}^n = \int \left( \prod_{\alpha<\beta} D q_{\alpha\beta}(x) \right) \exp(-\mathcal{H}_{\text{rep}}\{q_{\alpha\beta}\}). \tag{4}
\]

Here, \( q_{\alpha\alpha} = 0 \), we have omitted some unimportant terms of order \( q^4 \), and set \( \tau = 1 - T/T_c \). The fourth order term included is the one responsible for replica symmetry breaking. We assume that the dimension \( d \) is above the special dimension \( 8 \) to keep the loop expansion straightforward [6].

Since we are keeping \( n \) finite throughout, it will be necessary to review some of the results that have been derived in [3, 5, 7, 8, 10] for integer \( n \), allowing us to write, e.g., \( q_{\alpha\beta} \) with integer indices \( \alpha \) and \( \beta \), and of results that have been derived for arbitrary (noninteger) \( n \) and with an infinite number of symmetry breaking steps, such that we must re-write \( q_{\alpha\beta} \) in terms of \( q(x) \) where \( x \) is a continuous variable between \( n \) and 1. We will have to switch between these notations frequently but note that they are equivalent. In order to distinguish better between the cases \( n > 0 \) and \( n < 0 \), we will from now on use the notation \( n^+ \) for positive \( n \) and \( n^- \) for negative \( n \). The letter \( n \) itself will be used when no distinction is needed.
To Gaussian order we get from Eq. (4)
\[ \ln \Omega_n = -H_{\text{rep}}(q_{\alpha \beta}^{\text{SP}}) - \frac{V}{2} \int \frac{d^d k}{(2\pi)^d} \sum_\mu d_\mu \ln(k^2 + \lambda_\mu), \]
where $q_{\alpha \beta}^{\text{SP}}$ is the Parisi saddle point solution, $k$ is a $d$-dimensional wave vector and $\lambda_\mu, d_\mu$ are the eigenvalues of the Hessian, evaluated at the saddle point solution, and their degeneracies.

The first (mean field) term in Eq. (5) has been worked out by Kondor [7] for finite $n^+$. We repeat his calculation here for $n^-$ since it gives a qualitatively different result which we will need later on. The free energy at mean-field level for the Parisi function $q_n(x)$ at finite $n$ is (cf. Eq. (9) of [6])
\[ -\frac{H_{\text{rep}}}{n} = \frac{\tau}{2} \int_n^1 dx q_n^2(x) + \frac{y}{12} \int_n^1 dx q_n^4(x) - \frac{w}{6} \int_n^1 dx \left( x q_n^3(x) + 3q_n^2(x) \int_x^1 dt q_n(t) \right), \]
when extremized with respect to $q_n(x)$. The solutions for $n^+$ and $n^-$ are
\[ q_{n^+}(x) = \begin{cases} \frac{3w^+}{4y} & n^+ \leq x \leq 3n^+/2 \\ \frac{wx}{2y} & 3n^+/2 < x \leq x_1 \\ \frac{wx_1}{2y} & x_1 < x \leq 1 \end{cases}, \]
\[ q_{n^-}(x) = \begin{cases} 0 & n^- \leq x \leq 0 \\ \frac{wx}{2y} & 0 < x \leq x_1 \\ \frac{wx_1}{2y} & x_1 < x \leq 1 \end{cases}, \]
where $x_1 = 1 - \sqrt{1 - 4y^2/w^2}$ is the usual breakpoint of the Parisi $q$-function. Fig. 1 shows the two solutions for illustration.

We note that the kind of problem we are going to encounter already shows up at this level: $H_{\text{rep}}[q_{n^-}(x)]$ has no terms of higher order than $n^-$, while $H_{\text{rep}}[q_{n^+}(x)]$ does have additional terms of order $n^+6$ and higher [6]. We also note that at mean-field level, the variance $\Delta F^2$ is 0 since there is no $n^2$-term.

In order to calculate the fluctuation corrections, it is useful to define
\[ I = \sum_\mu d_\mu \ln(k^2 + \lambda_\mu). \]
By differentiating $I$ with respect to $k^2$ one obtains
\[ \frac{\partial I}{\partial (k^2)} = \sum_\mu \frac{d_\mu}{k^2 + \lambda_\mu} = \sum_{\alpha < \beta} G_{\alpha \beta, \alpha \beta}, \]
where $G_{\alpha \beta, \alpha \beta}$ are the propagators, which are essentially the inverse of the Hessian. The propagators have been calculated exactly by De Dominicis et al. [6] in the “continuum limit” of infinitely many replica symmetry breaking steps. While their results are too long to be quoted here, we mention that the diagonal propagators $G_{\alpha \beta, \alpha \beta}$ are in this limit denoted by $G_{\alpha \beta, \alpha \beta}^{xx}$, are labelled by a continuous variable $x \in [n, 1]$, and we have
\[ \sum_{\alpha < \beta} G_{\alpha \beta, \alpha \beta} = -\frac{n}{2} \int_n^1 dx G_{\alpha \beta, \alpha \beta}^{xx}. \]
For ease of notation, we will from now on drop the subscript 11 from the propagators (which is superfluous for our purposes) and replace it by $n$ to indicate that the propagators here still depend on it. While the propagators in [6] were derived for $n = 0$, it is possible but tedious to extend the calculation to finite $n$. Fortunately, there is a simple argument to obtain the propagators’ exact form for $n^-$. Since they are labelled by the variable $x$, which is nothing but the inverse of the Parisi function, i.e. $x(q)$, they are effectively labelled by $q$. From this we can infer that $G_{\alpha \beta, \alpha \beta}^{xx} = \text{const.}$ for those $x$ where $q_{n^-}(x)$ is a constant, therefore (cf. Eq. (8)) $G_{n^-}^{xx} = G_0^{xx}$ for $x \leq 0$, and for $x \geq 0$, $G_{n^-}^{xx} = G_0^{xx}$ because $q_{n^-}(x) = q_0(x)$. We can thus express the propagators for $n^-$ entirely in terms of the $n = 0$ propagators. For $n^+$ this simple argument does not work because $q_{n^+}(x)$ from Eq. (7) is (almost) identical to the $q$-function in a field, and it has been shown in [6] that this leads to an additional $n^+$-dependent term in the propagators. We will see below that luckily we do not need to work this out in detail.

We are now in a position to calculate $\Delta F^2$ for $n^-$. First, we calculate
\[ \frac{\partial I}{\partial (k^2)} = -\frac{n^-}{2} \int_n^1 dx G_{n^-}^{xx} = -\frac{n^-}{2} \int_n^1 dx G_0^{xx} + \frac{n^-}{2} G_0^{00}. \]
Thus there are no terms of higher order than $n^-2$. This already implies, by comparison with Eq. (9), that the free energy fluctuations have a Gaussian distribution since all higher order cumulants are zero. In order to calculate the variance of this distribution, $\Delta F^2$, we only need to know...
the coefficient of the \(n^{-2}\)-term, which is simply \(C_{00}^{(0)}\), and integrate it with respect to \(k^2\). The propagator \(C_{00}^{(0)}\) is given by \[ (13) \]

\[
C_{00}^{(0)} = \int_0^1 ds \int_0^1 dt \frac{\partial^2}{\partial s \partial t} f(s, t) - \int_0^1 \left( \frac{ds}{s} \frac{\partial}{\partial s} f(s, x_1) + \frac{dt}{t} \frac{\partial}{\partial t} f(x_1, t) \right) + f(x_1, x_1),
\]

where

\[
f(s, t) = \frac{1}{k^2 + yq^2(s) + yq^2(t)}
\]

is the inverse of the \(x = 0\) eigenvalues of the Hessian from the replicon sector \(\mathcal{B}\). The function \(f\) can easily be integrated with respect to \(k^2\), and the integrals in \(C_{00}^{(0)}\) can then be worked out, resulting in

\[
J := \int d(k^2)C_{00}^{(0)} = \ln(k^2 + \frac{x_1^2 u^2}{2g}) - \frac{4w(4yk^2 + wx_1)}{4yk^2 + 4y^2x_1^2} \tan^{-1} \frac{wx_1}{\sqrt{4yk^2 + w^2x_1^2}},
\]

such that

\[
\beta^2 \Delta F^2 = -\frac{V}{2} \int \frac{dt^4k}{(2\pi)^4} J.
\]

The integrals over \(k\) diverge unless we introduce a cutoff, which is tacitly implied in Eq. \[ (17) \].

According to what we found so far for \(n^-\), the free energy fluctuates with a Gaussian distribution and a variance as given by Eq. \[ (17) \]. This is, we believe, the physically sensible solution: if, by the usual argument, a spin glass sample is divided into many subsystems, each should contribute a random dominant bulk term and a subdominant surface term to the free energy, and by the central limit theorem this should give rise to a self-averaging, Gaussian-distributed quantity.

If we repeat the above procedure for \(n^+\), however, we find the following situation, which is illustrated most easily in a large-\(k^2\) expansion of the propagators \[ (1) \].

\[
G_{\alpha\beta, \alpha\beta} = \frac{1}{k^2} + \frac{2\tau + 2yq^2_{\alpha\beta}}{k^2} + \frac{1}{k^6} \left( (2\tau + 2yq^2_{\alpha\beta})^2 + w^2(q^2_{\alpha\alpha} + (q^2_{\beta\beta} - 2q^2_{\alpha\beta}) \right) + O(1/k^8).
\]

This expansion allows for a simple evaluation of \(\sum_{\alpha < \beta} G_{\alpha\beta, \alpha\beta}\), or rather \(-n/2 \int_0^1 dx G_{xx}^{xx}\), term by term. While the first two terms are identical for \(n^+\) and \(n^-\), the coefficient of the \(1/k^6\)-term is

\[
-\frac{n^+}{2}(4\tau^2 - 8y\tau q + \frac{w^4x^4}{4y^2}(1 - 4x_1/5)) + \frac{n^+}{2}(4\tau^2 - 2w^2q) - n^+ \frac{81w^4}{5 \cdot 128y^2},
\]

while for \(n^-\) one obtains the same but without a \(n^{-6}\)-term. Here we have used the abbreviation \(q = -f_{n} q^2_n(x) dx\), which is independent of \(n\). This shows that at least one expansion coefficient, and thus the physical consequences, changes when changing the sign of \(n\), since a nonzero \(n^6\)-term implies a non-gaussian probability distribution of the free energy.

The difference between the two cases \(n^+\) and \(n^-\) can be eliminated by modifying Parisi’s original symmetry breaking scheme for \(n^+\) in the following way. The \(q\)-matrix is divided into \(p\) boxes on the diagonal, each of which contains a Parisi-type symmetry broken matrix \(Q_{\alpha\beta}\), while the rest of the matrix is zero. This is illustrated in Eq. \[ (20) \] for \(p = 4\),

\[
q = \begin{pmatrix}
Q_{\alpha\beta} & & & \\
& Q_{\alpha\beta} & & \\
& & Q_{\alpha\beta} & \\
& & & Q_{\alpha\beta}
\end{pmatrix}.
\]

Now we first let the number of symmetry breaking steps \(R\) go to infinity, then we let \(p\) go to infinity, all the while keeping \(n^+\) finite.

This procedure is in fact very closely related to, but certainly not identical to, the original Parisi scheme. If we introduce the usual “integers” \(n^+ = m_0, m_1, \ldots, m_R, m_{R+1} = 1\) which characterise the block sizes of the symmetry broken matrix, then the difference between this scheme and the original one is that \(m_1 = n^+ / p\) is allowed to go to 0 before \(m_0\). This way of looking at it shows precisely where the difference between positive and negative \(n\) lies in the original scheme: for \(n^-\), \(m_1 \) does go to 0 before \(m_0\) since 0 now lies in the interval \([n^-, 1]\). It also shows that we may still use those exact results of \[ (3) \] for the modified scheme which were derived for arbitrary \(m\)’s.

From Eq. \[ (3) \] it follows now that on mean-field level, \(H_{\text{rep}}[q_{n^+}(x)]\) is to be replaced by \(pH_{\text{rep}}[q_{n^+ / p}(x)]\) (there are \(p\) Parisi blocks of size \(n^+ / p\) each), and in the limit \(p \to \infty\) this kills the \(n^{-6}\) and higher order terms in Kondor’s solution (terms of order \(n^{-m}\) are replaced by \(p(n^+ / p)^m \to 0\) \((p \to \infty)\) for \(m > 1\)), while only the term linear in \(n^+\) survives, unaltered. Thus this procedure has cured the inconsistency on the mean-field level without affecting the average free energy itself. It also cures the discrepancy on the Gaussian level, as the following argument shows. The eigenvalue equation for the
Hessian which follows from Eq. (3) is
\[(\lambda + 2\tau)f_{\alpha\beta} + w \sum_{\gamma} q_{\beta\gamma} f_{\gamma\alpha} + w \sum_{\delta} q_{\delta\alpha} f_{\beta\delta} + 2gq_{\alpha\beta} f_{\alpha\beta} = 0,\] (21)
where \(\lambda\) is the eigenvalue and \(f_{\alpha\beta}\) is the eigenvector. Since \(q_{\alpha\beta}\) is zero in the off-diagonal blocks, the eigenvectors can be chosen to be zero everywhere except in one block (and its counterpart on the opposite side of the diagonal, if the block does not happen to be on the diagonal). If \(f_{\alpha\beta}\) is nonzero in a block on the diagonal, the problem reduces to the eigenvalue problem of the original Parisi matrix, but of size \(n^+/p\). There are \(p\) blocks on the diagonal, i.e., we have to replace \(-\frac{n^+}{2} f_{n^+}^1 dx G_{n^+}^{xx}\) in Eq. (1) by \(-p\frac{n^+}{4p} \int_{n^+}^1 dx G_{n^+}^{xx}/p\), which again in the limit \(p \to \infty\) kills all terms of order \(n^+^2\) and higher but leaves the linear term unchanged. There are however additional eigenvectors which are nonzero in one of the off-diagonal blocks, of which there are \(p(p-1)/2\). According to [6, 8] the corresponding eigenvalues are again just the \(\alpha = 0\) eigenvalues from the replicon sector, given by \(1/f(s, t)\) from Eq. (14), and their contribution to \(\partial I/\partial (k^2)\) can once more be reduced to the propagator \(G_{00}^{00}\) and is \((p(p-1)/2)(n^+/p)^2 G_{n^+}^{00}/p \to (n^+^2/2)G_{00}^{00}\) (\(p \to \infty\)), while higher order terms vanish.

Collecting the pieces we get
\[
\frac{\partial I}{\partial (k^2)} = -\frac{n^+}{2} \int_0^1 dx G_{00}^{xx} + \frac{n^+^2}{2} G_{00}^{00}.\] (22)

Comparison with Eq. (12) shows that this modified type of symmetry breaking gives identical results to the ones derived before for \(n^-\) and thus eliminates the discrepancies between \(n^+\) and \(n^-\) limits.

The argument above also shows that the stability of the solution is not affected by the modification since all eigenvalues of the Hessian are the same as for the original scheme and are thus \(\geq 0\).

We conclude with a few remarks. A consequence of our modification of the symmetry breaking scheme is that the Parisi q-function is not well defined for \(n > 0\) since the numbers \(m_0, m_1, \ldots\) do not form a monotonous sequence any more. Instead, it turns into the multi-valued function sketched in Fig. 2, elegantly restoring symmetry with \(q_{n^-}(x)\), which was violated in Fig. 1. Integrals over functions \(g\) of \(q_{n^+}(x)\) have then to be interpreted as
\[
\int_{n^+}^1 dx g(q_{n^+}(x)) = \int_{n^+}^0 dx g(q_{n^-}^+(x)) + \int_{n^+}^1 dx g(q_{n^-}^-(x)),\] (23)
where the arrows denote the branch in an obvious way.

Physical quantities like the probability distribution of the order parameter, \(P(q) = dx dq\), are unaffected by this maneuver since they are only meaningful at \(n = 0\).

The need to modify Parisi’s original symmetry breaking to the scheme described here probably escaped notice as the two schemes become identical in the limiting case \(n = 0\), which is usually considered. Indeed higher order terms in the expansion in \(n\) have rarely been investigated for spin glasses as they are extremely difficult to compute when using the established \(n^+\)-formalism as in [6]. With our modified scheme, however, (or, equivalently, by working at \(n \to 0\)) not only are the higher order terms guaranteed to be correct but as shown here they also become relatively accessible. This may be important for future applications, e.g. for computing interface energies in spin glasses (see [1] for an attempt in this direction). We would also expect that the modification of the Parisi scheme described here is needed for the Sherrington-Kirkpatrick infinite range model. Whether this is the case or not could be investigated from the sample to sample fluctuations of the ground state energy of this model, which can be determined numerically when the number of spins \(N\) is small [2].

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References:

[1] G. Parisi, Phys. Lett. 73A, 203 (1979).
[2] G. Parisi, J. Phys. A 13, L115 (1980).
[3] G. Parisi, J. Phys. A 13, 1101 (1980).
[4] M. M´ ezard, G. Parisi, and M. A. Virasoro, Spin glass theory and beyond (World Scientific, Singapore, 1987).
[5] A. J. Bray and M. A. Moore, J. Phys. C 12, 79 (1979).
[6] C. De Dominicis, I. Kondor, and T. Temesv´ ari, in Spin glasses and random fields, edited by A. P. Young (World Scientific, Singapore London, 1997), no. 12 in Series on directions in condensed matter physics.
[7] I. Kondor, J. Phys. A 16, L127 (1983).
[8] T. Temesv´ ari, C. De Dominicis, and I. Kondor, J. Phys. A 27, 7569 (1994).
[9] C. De Dominicis, I. Kondor, and T. Temesv´ ari, J. Phys. I France 4, 1287 (1994).

FIG. 2: The multi-valued function \(q_{n^+}(x)\) for the modified symmetry breaking scheme. Note the similarity with \(q_{n^-}(x)\) from Fig. 1.
[10] C. De Dominicis, D. M. Carlucci, and T. Temesvári, J. Phys. I France 7, 105 (1997).
[11] T. Aspelmeier, M. A. Moore, and A. P. Young (2002), cond-mat/0209290.
[12] M. Palassini and A. P. Young (2002), unpublished.
[13] Expanding $I$ from Eq. (9) for large $k^2$ shows that it behaves like $\ln k^2 + O(1/k^2)$, i.e. there is no constant term of $O(1)$. This property determines the constant of integration and amounts to using the indefinite integral

$$\int d(k^2) f = \ln(k^2 + yq^2_0(s) + yq^2_0(t)).$$