An exact relation between free energy fluctuations and bond chaos in the Sherrington–Kirkpatrick model

T Aspelmeier
Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany
E-mail: aspel@theorie.physik.uni-goettingen.de

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Abstract. Using a variant of the interpolating Hamiltonian technique, we show that there exists, in the Sherrington–Kirkpatrick spin glass, an exact connection between the sample-to-sample fluctuations of the free energy and bond chaos involving two- and four-replica overlaps between replicas with different but correlated bonds. This relation is used to derive an upper bound of the fluctuations.

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1. Introduction

Extreme value statistics is a very active field in current mathematical physics since the discovery of the Tracy–Widom distribution for the largest (or smallest) eigenvalue of a Gaussian random matrix, see [1] for an overview. The Tracy–Widom distribution is believed to constitute a new universality class for extreme values in addition to the three ‘classical’ ones (Weibull, Gumbel and Fréchet). There are, however, many cases which do not fall into any of these four classes. One important example is the distribution of ground state energies in the Sherrington–Kirkpatrick model [2]. Despite tremendous numerical effort over the years [3]–[9], there is still no complete agreement as to what kind of distribution the ground states follow. Analytically, there is no theory (to the best of our knowledge) which would predict a particular limiting distribution for large system sizes $N$. Not even the width of the distribution is precisely known: the numerical simulations seem to suggest that the width scales as $N^\mu$ with $\mu \approx \frac{1}{4}$, and this is supported by some heuristic arguments [10, 4]. Other arguments favour $\mu = \frac{1}{6}$ [11, 12]. (If this problem fell into the Tracy–Widom universality class, the width would scale as $N^{1/3}$ [6]. This seems to be ruled out by the numerical results.)

In addition to the ground state energies and their sample-to-sample fluctuations one can also consider the sample-to-sample fluctuations of the free energy at a finite temperature within the spin glass phase. The natural expectation would be that in the low temperature phase these free energies fall into the same universality class as the ground state energies (although this has never been proved). However, the distribution of the free energies appears as inaccessible as the one of the ground state energies. Part of the difficulty lies in the fact that the variance of the distribution scales with a subextensive
power of $N$. In order to calculate subextensive terms, it is usually necessary to go to higher than the leading order in the loop expansion of the spin glass problem. Due to the massless modes present throughout the spin glass phase this has so far been impossible in the Sherrington–Kirkpatrick model. For the finite-dimensional spin glass, this problem is not so severe and the fluctuations could be calculated \[13,14\]. They are, however, fundamentally different from the ones in the Sherrington–Kirkpatrick model, which we will be considering here.

In this paper we present a way which circumvents this obstacle by constructing an exact relation between the free energy fluctuations and bond chaos in spin glasses. This connection has been briefly described in \[15\] and we present the details of the calculation here. Using this relation, the width of the distribution can, in principle, be calculated by calculating chaos. A part of the necessary aspects of chaos has been calculated in \[16\] and the results from that paper will be sufficient to derive the upper bound \(\mu \leq \frac{1}{4}\) here. For the full answer, it will be necessary to calculate more complicated objects such as simultaneous four-replica overlaps. We will not be able to solve this formidable problem here.

This paper is organized as follows. In section 2 we briefly review a few methods and results from the literature in order to compare them with our own theory later on. We derive the connection to bond chaos in section 3. The fluctuations above and at the critical temperature, as well as the bound \(\mu \leq \frac{1}{4}\) in the low temperature phase, are calculated in section 4. We end with a conclusion in section 5.

### 2. Above and at the critical temperature

In this section we review a few methods and results above and at the critical temperature from the literature for completeness and for comparison with our own results later on.

Analytically, the free energy fluctuations of any disordered system can in principle be found with the replica method. Given the partition function $Z$ of a system of size $N$, it can easily be shown that a Taylor expansion of $\log Z$ in powers of $n$ yields

$$\log Z^n = -n\beta F_N + \frac{n^2}{2} \Delta F_N^2 + \cdots,$$

(1)

where the overbar means the average over the disorder, $\beta = 1/k_B T$ is the inverse temperature, $F_N$ is the average free energy at system size $N$ and $\Delta F_N$ denotes its sample-to-sample fluctuations. The dots indicate higher-order cumulants. Using the replica formalism, one can calculate $Z^n$ for integer $n$ and try to continue the resulting expression to real (or, indeed, complex) $n$ and isolate the coefficient of the second-order term which represents the fluctuations. In the case of the Ising spin glass this works very nicely above and at the critical temperature. It is straightforward to show with the standard replica formalism for the mean-field spin glass \[17\] that in the high temperature phase ($\beta < 1$), where the saddle point is replica symmetric and its Hessian has only strictly positive eigenvalues, the fluctuations are

$$\beta^2 \Delta F_N^2 = -\frac{1}{2} \log(1 - \beta^2) - \frac{\beta^2}{2} + O(1/N)$$

(2)

[11,18]. As the critical temperature $T_c$ is approached ($\beta \nearrow 1/T_c = 1$), this expression diverges, which indicates that the fluctuations at the critical point must also diverge.
Free energy fluctuations and bond chaos

with $N$. A straightforward extension of the calculation in [18] shows that the fluctuations at the critical point are

$$
\beta^2 \Delta F_N^2 = \frac{1}{6} \log N + O(1),
$$

which does indeed diverge as $N \to \infty$. As a check, we can rederive this result from equation (2) by isolating the divergent part, $-\frac{1}{2} \log (1 - \beta)$, and replacing $1 - \beta \sim \tau$ (where $\tau = (T - T_c)/T_c$ is the reduced temperature) by $x N^{-1/3}$. The variable $x = \tau N^{1/3}$ is the correct scaling combination in the critical region [18, 19]. Keeping $x$ fixed and letting $N$ tend to infinity in $-\frac{1}{2} \log (x N^{-1/3})$ results in equation (3).

In the low temperature phase, the situation is much more complex and there are no reliable analytical results.

3. Interpolating Hamiltonian

In this section we will derive two different exact expressions for the fluctuations in terms of chaos using interpolating Hamiltonians. While the calculation presented here is in spirit similar to the one by Billoire [20], there is an important difference. Here, we do not interpolate between a big system and two small systems (see also [21]) but between two equally big systems. This may seem strange at first sight but is in fact the key to making any analytical progress on this particular problem.

3.1. First route to chaos

Consider the following interpolating Hamiltonian:

$$
\mathcal{H}_t = -\sqrt{\frac{1-t}{N}} \sum_{i<j} J_{ij} s_is_j - \sqrt{\frac{t}{N}} \sum_{i<j} J'_{ij} s_is_j,
$$

with $N$ Ising spins $s_i$, $0 \leq t \leq 1$ and $J_{ij}$, $J'_{ij}$ independent Gaussian random variables with unit variance. The parameter $t$ interpolates between one spin glass system ($t = 0$) and a statistically independent, but otherwise identical, one at $t = 1$. It is important to note that also for each other value of $t$ the Hamiltonian describes a normal spin glass, the coupling constants being $\sqrt{1-t} J_{ij} + \sqrt{t} J'_{ij}$ which are Gaussian random variables with unit variance.

The partition function of this Hamiltonian is $Z_t = \text{Tr} \exp(-\beta \mathcal{H}_t)$ and the free energy is $\beta F_t = -\log Z_t$. The sample-to-sample fluctuations of the free energy of the SK model can be obtained in the following way. Denoting the average over all coupling constants $J_{ij}$ and $J'_{ij}$ (and later also $J''_{ij}$ and others) by $\langle \cdots \rangle$, we have

$$
E (\log Z_1 - \log Z_0)^2 = \beta^2 E (F_1 - F_0)^2
$$

$$
= \beta^2 (E F_1^2 - 2E F_1 F_0 + E F_0^2)
$$

$$
= 2\beta^2 (E F_1^2 - F_1^2)
$$

$$
= 2\beta^2 \Delta F_1^2.
$$

The penultimate step follows from the fact that $E F_1^2 = E F_0^2 = \overline{F^2}$ is the disorder average of the squared spin glass free energy and that the average $E F_1 F_0 = (E F_1)(E F_0) = : F_1^2$
factorizes into the square of the averaged free energy since the coupling constants in the two
Hamiltonians $H_0$ and $H_1$ are independent. Using this formulation and the idea developed
in [21] to represent $\log Z_1 - \log Z_0$ by differentiating with respect to the interpolation
parameter $t$ and immediately integrating again, the fluctuations can be written as

$$2\beta^2\Delta F^2_k = E(\log Z_1 - \log Z_0)^2 = \int_0^1 dt \int_0^1 d\tau E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau. \quad (9)$$

In the appendix it is shown how to manipulate this expression in order to arrive at
equation (A.14), which is repeated here for convenience. Note that this equation is exact:

$$E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = \frac{N^2\beta^4}{16} \left(2 - \sqrt{1-t} \sqrt{\tau} - \sqrt{1-\tau} \sqrt{1-t}\right) E \langle(q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2)\rangle + \frac{N\beta^2}{4\sqrt{\tau}} \left(E \langle q_{13}^2 \rangle - \frac{1}{N}\right). \quad (10)$$

The symbols $q_{ab}$ are overlaps between independent replicas with different interpolation
parameters:

$$q_{ab}(t, \tau) = \frac{1}{N} \sum_i s_i^{a,t} s_i^{b,\tau}. \quad (11)$$

In equation (10) replicas 1 and 2 have parameter $t$ and replicas 3 and 4 have parameter $\tau$. The angular brackets $\langle \cdots \rangle$ denote the thermal average of a system of independent replicas
with the appropriate interpolation parameters.

We have thus established a connection between the fluctuations and the overlap between
replicas with different interpolation parameters. The last important step is to realize that, for any given value of $t$, $H_t$ represents a normal mean-field spin glass
with Gaussian couplings just like any other. The overlap $q_{13}$ between two replicas with
different interpolation parameters is therefore an overlap between two normal spin glasses
with identical bonds (if $t = \tau$), uncorrelated bonds (if $t = 0$, $\tau = 1$ or vice versa) or related,
but not equal bonds (for anything in between). This immediately shows the connection to chaos in spin glasses. Chaos concerns the question how the equilibrium states of two
initially equal systems are related when a small perturbation is applied to one of them,
e.g. a small change of temperature (temperature chaos) or a perturbation of the bonds
(bond chaos). When there is chaos, the equilibrium states are completely unrelated and
the overlap is 0 (in the thermodynamic limit), no matter how small the perturbation. In
our case, we are dealing with bond chaos.

Let $t$ and $\tau$ be given and let the coupling constants of $H_t$ be the reference configuration
of bonds: $K^0_{ij} := \sqrt{1-\tau} J_{ij} + \sqrt{\tau} J'_{ij}$. The coupling constants belonging to $H_\tau$ are
$K_{ij} = \sqrt{1-\tau} J_{ij} + \sqrt{\tau} J'_{ij}$. Since the $J_{ij}$ and $J'_{ij}$ are Gaussian random variables, so are $K^0_{ij}$
and $K_{ij}$ (also with unit variance). Their correlation is $E_{J,J'}K^0_{ij}K_{ij} = \sqrt{1-t}\sqrt{1-\tau} + \sqrt{t\tau}$. Instead of using $J_{ij}$ and $J'_{ij}$ as the basic independent random variables one could also use
$K^0_{ij}$, introduce new Gaussian random variables $K'_{ij}$ and take $K^0_{ij}$ and $K'_{ij}$ as the building
blocks of the random variables. We can then write the bonds pertaining to $H_\tau$ as

$$K_{ij}(\epsilon) = \frac{K^0_{ij}}{\sqrt{1+\epsilon^2}} + \frac{\epsilon K'_{ij}}{\sqrt{1+\epsilon^2}}. \quad (12)$$

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such that the correlation between $K^0_{ij}$ and $K_{ij}(\epsilon)$ is $E K^0_{ij} K_{ij}(\epsilon) = 1/\sqrt{1 + \epsilon^2}$. In order that the bonds $K_{ij}(\epsilon)$ are statistically equivalent to the original bonds of $\mathcal{H}_\tau$, the correlation must be equal to the correlation obtained before, so

$$\frac{1}{\sqrt{1 + \epsilon^2}} = \sqrt{1 - t\sqrt{1 - \tau}} + \sqrt{t\tau}. \quad (13)$$

Thus we see that the disorder average of the overlap $q_{ij}(t, \tau)$ is only a function of $\epsilon$, i.e. $E \langle q_{13}^2(t, \tau) \rangle = E \langle q_{13}^2(\epsilon) \rangle$ is only a function of $\epsilon$, not of $t$ and $\tau$ independently. The same applies, of course, for products of overlaps such as $E \langle q_{13}^2(t, \tau) q_{23}^2(t, \tau) \rangle = E \langle q_{13}^2(\epsilon) q_{23}^2(\epsilon) \rangle$.

The parameter $\epsilon$ can be interpreted as a ‘distance’ between the sets of bonds $\{K^0_{ij}\}$ and $\{K_{ij}(\epsilon)\}$ since at $\epsilon = 0$ the bonds are identical and have zero separation in the space of coupling constants, while at $\epsilon = \infty$ they are statistically independent, i.e. as far apart as they possibly can in a statistical sense.

In order to obtain the fluctuations, we must integrate equation (10) over $t$ and $\tau$, according to equation (9). But since the overlaps only depend on $\epsilon$, it is useful to make a variable substitution and go over to $\epsilon$ and $z := \sqrt{1 + \epsilon^2}/\sqrt{\tau}$. We first note that the integral $\int_0^1 dt \int_0^1 d\tau \cdots$ can be restricted to the range $\tau \leq t$ due to symmetry, provided a factor of 2 is inserted. We can then make the substitution and obtain

$$\beta^2 \Delta F^2_N = -\frac{N^2 \beta^4}{16} \int_0^\infty d\epsilon \, f_1(\epsilon) E \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle$$

$$+ \frac{N \beta^2}{4} \int_0^\infty d\epsilon \, g_1(\epsilon) \left( E \langle q_{13}^2 \rangle - \frac{1}{N} \right), \quad (14)$$

where

$$f_1(\epsilon) = \int_0^1 dz \, \mathcal{J} \left( \frac{\sqrt{1 - t} \sqrt{\tau}}{\sqrt{\tau} \sqrt{1 - \tau}} + \frac{\sqrt{1 - \tau} \sqrt{t}}{\sqrt{\tau} \sqrt{1 - t}} - 2 \right), \quad (15)$$

$$g_1(\epsilon) = \int_0^1 dz \, \mathcal{J} \frac{1}{\sqrt{t\tau}}, \quad (16)$$

with the Jacobian

$$\mathcal{J} = \frac{4z}{(1 + \epsilon^2)^4} (\epsilon \sqrt{1 + \epsilon^2 - z^2} + z)(\sqrt{1 + \epsilon^2 - z^2} - \epsilon z). \quad (17)$$

The old variables $t$ and $\tau$, expressed in terms of the new ones, are

$$t = \left( \frac{\epsilon \sqrt{1 + \epsilon^2 - z^2} + z}{1 + \epsilon^2} \right)^2, \quad (18)$$

$$\tau = \frac{z^2}{1 + \epsilon^2}. \quad (19)$$

The integrals in equations (15) and (16) can be evaluated explicitly and we find

$$f_1(\epsilon) = \frac{4\epsilon^2}{(1 + \epsilon^2)^2} \arcsin \frac{1}{\sqrt{1 + \epsilon^2}}, \quad (20)$$

$$g_1(\epsilon) = \frac{2}{(1 + \epsilon^2)^{3/2}} \arcsin \frac{1}{\sqrt{1 + \epsilon^2}}. \quad (21)$$

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Equation (14) is our first important result. It is exact and connects the fluctuations with bond chaos. If it were possible to calculate bond chaos (and it was shown in [16] that at least for the two-replica overlaps it is possible), the fluctuations follow immediately since the functions \( f_1(\epsilon) \) and \( g_1(\epsilon) \) are ‘harmless’ (equations (20) and (21)). Note that \( f_1(\epsilon) \) and \( g_1(\epsilon) \) are nonnegative and \( \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle \) is also nonnegative (this is shown in the appendix). The first term in equation (14) is therefore negative. Hence the second term is an upper bound for the fluctuations.

3.2. Second route to chaos

There is another way to represent the fluctuations with interpolating Hamiltonians than equation (8) which will lead to a second expression for the fluctuations. Introducing the Hamiltonian \( \mathcal{H}'_t \) defined by

\[
\mathcal{H}'_t = -\sqrt{\frac{1-t}{N}} \sum_{i<j} J_{ij} s_i s_j - \sqrt{\frac{t}{N}} \sum_{i<j} J''_{ij} s_i s_j,
\]

which only differs from \( \mathcal{H}_t \) by the second set of coupling constants \( J''_{ij} \) which are again independent Gaussian random variables with unit variance, we can write

\[
E (\log Z_1 - \log Z_0)(\log Z'_1 - \log Z'_0) = \beta^2 E (F_1 - F_0)(F'_1 - F'_0) = \beta^2 E (F_1 F'_1 - F_1 F'_0 - F_0 F'_1 + F_0 F'_0) = \beta^2(\overline{F^2} - \overline{F^2}) = \beta^2 \Delta F^2_N,
\]

where \( Z'_1 \) and \( F'_1 \) are the partition function and the free energy pertaining to \( \mathcal{H}'_t \). The fluctuations can be represented by a double integral, as above:

\[
\beta^2 \Delta F^2_N = \int_0^1 dt \int_0^1 d\tau E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z'_\tau.
\]

Proceeding precisely as above and in the appendix, we get

\[
E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z'_\tau = \frac{N^2 \beta^4}{16} E \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{8 \sqrt{1-t} \sqrt{1-\tau}} \left( E \langle q_{13}^2 \rangle - \frac{1}{N} \right).
\]

Replicas 1 and 2 have Hamiltonian \( \mathcal{H}_t \) and replicas 3 and 4 have \( \mathcal{H}'_t \).

Integrating over \( t \) and \( \tau \) gives us the fluctuations, and again the overlaps do not depend on \( t \) and \( \tau \) separately but only on the distance \( \epsilon \). The distance is here not given by equation (13) but is slightly different due to the independence of \( J' \)s and \( J'' \)s. Arguing similarly as above, \( \epsilon \) is found to be related to \( t \) and \( \tau \) by

\[
\frac{1}{\sqrt{1+\epsilon^2}} = \sqrt{1-t} \sqrt{1-\tau}.
\]
Making a change of variables to eliminate $\tau$ in favour of $\epsilon$ yields
\[
\beta^2 \Delta F_N^2 = \frac{N^2 \beta^4}{16} \int_0^\infty d\epsilon \int_0^{\epsilon^2/(1+\epsilon^2)} dt \frac{2\epsilon}{(1-t)(1+\epsilon^2)^2} E(q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2)
+ \frac{N\beta^2}{8} \int_0^\infty d\epsilon \int_0^{\epsilon^2/(1+\epsilon^2)} dt \frac{2\epsilon}{(1-t)(1+\epsilon^2)^2} \sqrt{1+\epsilon^2} \left(E(q_{13}^2) - \frac{1}{N}\right),
\]
such that
\[
\beta^2 \Delta F_N^2 = \frac{N^2 \beta^4}{16} \int_0^\infty d\epsilon f_2(\epsilon) E(q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) + \frac{N\beta^2}{4} \int_0^\infty d\epsilon g_2(\epsilon) \left(E(q_{13}^2) - \frac{1}{N}\right).
\]
This is the second result for the fluctuations. It has precisely the same structure as equation (14). The only difference are the weight functions under the integrals, which are given by
\[
f_2(\epsilon) = \frac{2\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^2},
\]
and
\[
g_2(\epsilon) = \frac{\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^{3/2}},
\]
and the sign of the first term, which is positive here.

4. Calculation of the fluctuations

Having established the connection to chaos, we can proceed to calculate the fluctuations by calculating $E(q_{13}^2)$ and $E(q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2)$. The former can be accomplished by taking the bond averaged probability distribution $P_\epsilon(q)$ of the overlap $q$ for bond chaos, which has been calculated in [16]. Averages taken with this probability distribution will be denoted by $\langle \cdots \rangle_0$. The latter is more difficult and will be postponed to a later publication. It requires the joint probability distributions $P_\epsilon^{123}(q_{13}, q_{23})$ and $P_\epsilon^{1234}(q_{13}, q_{24})$. However, above and at the critical temperature, there is no replica symmetry breaking, hence these probability distributions factorize into $P_\epsilon^{123}(q_{13}, q_{23}) = P_\epsilon(q_{13})P_\epsilon(q_{23})$ and $P_\epsilon^{1234}(q_{14}, q_{23}) = P_\epsilon(q_{14})P_\epsilon(q_{23})$ such that
\[
E(q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) = [q^4]_0 - [q^2]_0^2.
\]
We will be able to calculate this. Below the critical temperature, on the other hand, we will have to content ourselves with an upper bound of the fluctuations which is given by the second integral in equation (14).

4.1. Above the critical temperature

The nonnormalized probability distribution of the overlap $q$ for bond chaos, $R_\epsilon(q)$, above the critical temperature is [16]
\[
R_\epsilon^0(q) = e^{-N((q^2/2)h(\epsilon)+O(q^4))},
\]
with $h(\epsilon) = 1 - \beta^2/(\sqrt{1+\epsilon^2})$.

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For large $N$, we can easily calculate $[q^2]_0$ and $[q^4]_0$ via steepest descents. At leading order, the terms of order $q^4$ and higher in the exponent do not contribute. Defining $q_n := \int_0^\infty dq q^n R_\epsilon(q)$ (the upper bound may be set to $\infty$ as this only introduces exponentially small errors), we get

$$q_n = \frac{1}{2} \left( \frac{N}{2} h(\epsilon) \right)^{-(n+1)/2} \Gamma \left( \frac{n + 1}{2} \right), \quad (36)$$

such that

$$[q^2]_0 = \frac{q^2}{q_0} = \frac{1}{Nh(\epsilon)}, \quad (37)$$

$$[q^4]_0 = \frac{q^4}{q_0} = \frac{3}{N^2 h^2(\epsilon)}. \quad (38)$$

This allows us to write down two equations for the fluctuations from our two routes to chaos, equations (14) and (31), namely

$$\beta^2 \Delta F^2_N = -\frac{\beta^4}{8} \int_0^\infty d\epsilon \frac{f_1(\epsilon)}{h^2(\epsilon)} + \frac{\beta^2}{4} \int_0^\infty d\epsilon \frac{g_1(\epsilon)}{h(\epsilon)} \left( \frac{1}{h(\epsilon)} - 1 \right) \quad (39)$$

$$= \frac{\beta^4}{8} \int_0^\infty d\epsilon \frac{f_2(\epsilon)}{h^2(\epsilon)} + \frac{\beta^2}{4} \int_0^\infty d\epsilon \frac{g_2(\epsilon)}{h(\epsilon)} \left( \frac{1}{h(\epsilon)} - 1 \right). \quad (40)$$

The second of these expressions can be evaluated explicitly, with the result

$$\beta^2 \Delta F^2_N = -\frac{1}{2} \log(1 - \beta^2) - \frac{\beta^2}{2}, \quad (41)$$

in accordance with equation (2). The author is currently unable to calculate the integrals in equation (39) but numerical checks show that they give precisely the same result.

### 4.2. At the critical temperature

The nonnormalized probability distribution $R_\epsilon(q)$ precisely at the critical temperature is given by [16]

$$R_\epsilon(q) = \begin{cases} 
    e^{-Nw q^3/6} & \epsilon \ll N^{-1/6} \\
    e^{-Nq^2 h(\epsilon)/2} & N^{-1/6} \ll \epsilon.
\end{cases} \quad (42)$$

Define as before $q_n = \int_0^\infty dq q^n R_\epsilon(q)$. Then we find

$$q_n = \begin{cases} 
    \frac{1}{3} \left( \frac{Nw}{6} \right)^{-(n+1)/3} \Gamma \left( \frac{n + 1}{3} \right) & \epsilon \ll N^{-1/6} \\
    \frac{1}{2} \left( \frac{N}{2} h(\epsilon) \right)^{-(n+1)/2} \Gamma \left( \frac{n + 1}{2} \right) & N^{-1/6} \ll \epsilon.
\end{cases} \quad (43)$$
such that

$$[q^2]_0 = \frac{q_0^2}{q_0} = \begin{cases} \left( \frac{N w}{6} \right)^{-2/3} \frac{1}{\Gamma(1/3)} & \epsilon \ll N^{-1/6} \\
\frac{N}{2} h(\epsilon)^{-1} \frac{\Gamma(3/2)}{\Gamma(1/2)} & N^{-1/6} \ll \epsilon \end{cases}$$

(44)

and

$$[q^4]_0 = \frac{q_4}{q_0} = \begin{cases} \left( \frac{N w}{6} \right)^{-4/3} \frac{\Gamma(5/3)}{\Gamma(1/3)} & \epsilon \ll N^{-1/6} \\
\frac{N}{2} h(\epsilon)^{-2} \frac{\Gamma(5/2)}{\Gamma(1/2)} & N^{-1/6} \ll \epsilon. \end{cases}$$

(45)

Now we can evaluate equation (31). Plugging $[q^2]_0$ into the second term of that equation yields a constant of the order of 1 which is not of interest and will therefore not be calculated explicitly. The first term, however, is important. Splitting the integral into two parts we get asymptotically

$$\frac{N^2 \beta^4}{16} \int_0^{\infty} d\epsilon f_2(\epsilon) ([q^2]_0^2 - [q^2]_0^4) = \frac{N^2 \beta^4}{16} \int_0^{N^{-1/6}} d\epsilon f_2(\epsilon) \frac{\Gamma(5/3) \Gamma(1/3) - 1}{\Gamma^2(1/3)} \left( \frac{N w}{6} \right)^{-4/3} \Gamma(1/3) + \frac{N^2 \beta^4}{16} \int_{N^{-1/6}}^{\infty} d\epsilon f_2(\epsilon) \frac{1}{2} \left( \frac{N}{2} h(\epsilon) \right)^{-2}.$$  

(46)

The first of these integrals yield a constant (independent of $N$). The second one, however, gives a logarithm at the lower bound such that we get (with $f_2(\epsilon) = 2\epsilon^3 + O(\epsilon^5)$, $h(\epsilon) = \epsilon^2/2 + O(\epsilon^4)$ and $\beta = 1$ as we are at the critical point)

$$\beta^2 \Delta F_N^2 = \frac{1}{6} \log N + O(1).$$

(47)

This is precisely the known result.

It is interesting to note that we would not have been able to obtain this result so easily from our first route to chaos, equation (14), as both integrals in that expression grow with some power of $N$, and only their difference cancels out the leading behaviour and leaves a logarithmic divergence. In order to actually calculate this, we would need subleading corrections to the integrals, which would be very hard to obtain indeed.

4.3. Below the critical temperature

Now we turn to the low temperature phase. We will not be able here to solve the complete problem since $P_{\epsilon}^{123}(q_{13}, q_{23})$ and $P_{\epsilon}^{1234}(q_{14}, q_{23})$ do not factorize in the symmetry breaking phase. In [22, 23] it has been shown how to break down these probability distributions but the results only apply for $\epsilon = 0$. Instead, we focus on the second term in equation (14) since it only requires $P_{\epsilon}(q_{13})$ and provides an upper bound for the fluctuations.

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From [16] we get the nonnormalized probability distribution of $q$ in the low temperature phase, which is

$$R_n(q) = \begin{cases} 
\hat{\theta}(q - q_{EA}) & \epsilon \ll N^{-1/2} \\
e^{-Nc_1 \epsilon^2 q^3} & N^{-1/2} \ll \epsilon \ll N^{-1/5} \\
e^{-Nc_2 \epsilon^3 q^2} & N^{-1/5} \ll \epsilon \leq \epsilon_0 \\
e^{-NF(\epsilon)q^2} & \epsilon_0 < \epsilon,
\end{cases}$$

(48)

where

$$\hat{\theta}(x) = \begin{cases} 
1 & x < 0 \\
e^{-Nc_0 x^3} & x > 0,
\end{cases}$$

(49)

with some (unimportant) positive constant $c_0$ and $q_{EA}$ is the Edwards–Anderson order parameter, such that

$$q_n = \begin{cases} 
\frac{q_{EA}^{n+1}}{n+1} & \epsilon \ll N^{-1/2} \\
\frac{1}{3}(Nc_1 \epsilon^2)^{-(n+1)/3} \Gamma\left(\frac{n+1}{3}\right) & N^{-1/2} \ll \epsilon \ll N^{-1/5} \\
\frac{1}{2}(Nc_2 \epsilon^3)^{-(n+1)/2} \Gamma\left(\frac{n+1}{2}\right) & N^{-1/5} \ll \epsilon \leq \epsilon_0 \\
\frac{1}{2}(NF(\epsilon))^{-(n+1)/2} \Gamma\left(\frac{n+1}{2}\right) & \epsilon_0 < \epsilon
\end{cases}$$

(50)

and

$$[q^2]_0 \propto \begin{cases} 
\text{const.} & \epsilon \ll N^{-1/2} \\
(N\epsilon^2)^{-2/3} & N^{-1/2} \ll \epsilon \ll N^{-1/5} \\
(N\epsilon^3)^{-1} & N^{-1/5} \ll \epsilon \leq \epsilon_0 \\
(NF(\epsilon))^{-1} & \epsilon_0 < \epsilon.
\end{cases}$$

(51)

Note the discussion in [16] about why the probability distribution for $\epsilon \ll N^{-1/2}$ does not coincide with the true distribution for the Sherrington–Kirkpatrick model. However, this discrepancy only changes the value of $[q^2]_0$ for small $\epsilon$. It does not change the qualitative behaviour of $[q^2]_0$ as a function of $\epsilon$.

We can estimate the integral $(N\beta^2/4) \int_0^\infty d\epsilon g_1(\epsilon)(E\langle q_{13}^2 \rangle - 1/N)$ from equation (14) by first neglecting the $1/N$ term under the integral as we are only interested in the leading behaviour. We can also neglect the contribution of the integration from $\epsilon_0$ to $\infty$ since it will only be of the order of 1. We also note that we can combine the regions $\epsilon \ll N^{-1/2}$ and $N^{-1/2} \ll \epsilon \ll N^{-1/5}$ by writing $[q^2]_0 = F(1/N^2\epsilon)$ with a scaling function $F(x)$ with the properties $F(x) \to \text{const.} (x \to 0)$ and $F(x) \sim x^{-4/3} (x \to \infty)$. We then obtain for the first part of the integral (expanding the function $g_1(\epsilon)$ for small $\epsilon$)

$$\frac{N\beta^2}{4} \int_0^{N^{-1/5}} d\epsilon g_1(\epsilon)[q^2]_0 \approx \frac{N\beta^2}{4} \pi \int_0^{N^{-1/5}} d\epsilon F(1/N^2\epsilon)
= N^{1/2} \frac{\beta^2}{4} \pi \int_0^{N^{3/10}} dx F(x) \sim N^{1/2}.$$
The next part of the integral is
\[ \frac{N\beta^2}{4} \int_{N^{-1/5}}^{\epsilon_0} d\epsilon g_1(\epsilon) [q^2]_0 \sim \frac{N\beta^2}{4} \pi \int_{N^{-1/5}}^{\epsilon_0} \frac{1}{N\epsilon^8} \sim N^{2/5}. \] (53)

This contribution is smaller than the one we just had and may be neglected.

The final answer for the fluctuations in the low temperature phase is therefore
\[ \beta^2 \Delta F_N^2 \leq \text{const.} \times N^{1/2}, \] (54)
i.e. we get the upper bound
\[ \mu \leq \frac{1}{4}. \] (55)

### 5. Conclusion

We have shown that the free energy fluctuations in the Sherrington–Kirkpatrick model can be expressed in two different ways in terms of bond chaos, equations (14) and (31), both of which are exact. The first formulation consists of a difference of two positive terms while the second is a sum of positive terms. We have derived an upper bound of the fluctuations using the first formulation, resulting in \( \mu \leq \frac{1}{4} \). In the future, the second formulation will be more useful because it allows direct access to the fluctuations when four-replica overlaps are calculated, either numerically or analytically, since it is easy to see that the second integral in equation (31) is subdominant and only the first integral needs to be evaluated in order to obtain the leading behaviour of the fluctuations.

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### Appendix. Evaluation of the interpolating Hamiltonians

In this appendix we show the details of the derivation of the connection to chaos. The partial derivatives in equation (9) evaluate to
\[ \frac{\partial}{\partial t} \log Z_t = \frac{1}{Z_t} \Tr \left( \frac{\beta}{2\sqrt{t\sqrt{N}}} \sum_{i<j} J'_{ij} s_is_j - \frac{\beta}{2\sqrt{1-t\sqrt{N}}} \sum_{i<j} J_{ij} s_is_j \right) \exp(-\beta\mathcal{H}_t) \] (A.1)
\[ = \frac{1}{2t} \sum_{i<j} J'_{ij} \frac{\partial \log Z_t}{\partial J'_{ij}} - \frac{1}{2(1-t)} \sum_{i<j} J_{ij} \frac{\partial \log Z_t}{\partial J_{ij}}. \] (A.2)

It remains to deal with the average over the disorder in
\[ E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = E \sum_{i<j,k<l} \left( \frac{1}{2t} J'_{ij} \frac{\partial \log Z_t}{\partial J'_{ij}} - \frac{1}{2(1-t)} J_{ij} \frac{\partial \log Z_t}{\partial J_{ij}} \right) \times \left( \frac{1}{2\tau} J'_{kl} \frac{\partial \log Z_\tau}{\partial J'_{kl}} - \frac{1}{2(1-\tau)} J_{kl} \frac{\partial \log Z_\tau}{\partial J_{kl}} \right). \] (A.3)

Let us look at the first term of the product under the sum, \( E (1/4t\tau) J'_{ij} J'_{kl} (\partial \log Z_t/\partial J'_{ij}) (\partial \log Z_\tau/\partial J'_{kl}) \). We can integrate by parts with respect to, say, \( J'_{ij} \) (a
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The standard trick [21] in the form

\[ E \left. J'_{ij} J'_{kl} \right| = \int \cdots \prod \left. J'_{ij} e^{-J'_{ij}^2/2} \right. \cdots J'_{ij} J'_{kl} \right| = \int \cdots \prod \left. J'_{ij} e^{-J'_{ij}^2/2} \right. \cdots = E \frac{\partial}{\partial J_{ij}} J'_{kl} \right| , \tag{A.4} \]

where the \( \bullet \) stands symbolically for any function of the \( J_{ij} \) and \( J'_{ij} \). The derivative can be moved to the right using the product rule so

\[ E \left. J'_{ij} J'_{kl} \right| = E \left( \delta_{(ij),(kl)} + J'_{kl} \frac{\partial}{\partial J_{ij}} \right) \bullet . \tag{A.5} \]

Here, the second term can once again be treated by integration by parts, this time with respect to \( J'_{kl} \). The result is

\[ E \left. J'_{ij} J'_{kl} \right| = E \left( \delta_{(ij),(kl)} + \frac{\partial}{\partial J_{kl}'} \frac{\partial}{\partial J_{ij}'} \right) \bullet . \tag{A.6} \]

The same procedure can be applied to the remaining terms in equation (A.3), with the difference that the terms that mix \( J \) and \( J' \) do not have the \( \delta_{(ij),(kl)} \), resulting in

\[
E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = E \sum_{i<j<k<l} \left[ \frac{1}{4t\tau} \frac{\partial}{\partial J_{kl}'} \frac{\partial}{\partial J_{ij}'} \frac{\partial}{\partial J_{ij}'} \frac{\partial}{\partial J_{kl}'} \frac{\partial}{\partial J_{ij}'} \frac{\partial}{\partial J_{ij}'} \frac{\partial}{\partial J_{kl}'} \frac{\partial}{\partial J_{ij}'} \right] \left( \delta_{(ij),(kl)} + \frac{\partial}{\partial J_{kl}'} \frac{\partial}{\partial J_{ij}'} \right) \bullet . \tag{A.7} \]

The derivatives which appear in this expression are related to spin averages. One finds, for example,

\[ \frac{\partial \log Z_t}{\partial J_{ij}} = \frac{\beta}{\sqrt{N}} \sqrt{1-t} \langle s_i s_j \rangle_t , \tag{A.8} \]

where \( \langle \cdots \rangle_t \) stands for the thermal average, to be taken with the interpolation parameter set to \( t \). Similarly, for two derivatives, one obtains, for instance,

\[
\frac{\partial^2 \log Z_t}{\partial J_{ij} \partial J'_{kl}} = \frac{\beta^2}{N} \sqrt{1-t} \sqrt{1} \left( \langle s_i s_j s_k s_l \rangle_t - \langle s_i s_j \rangle_t \langle s_k s_l \rangle_t \right) . \tag{A.9} \]

In general, each derivative with respect to a \( J \) or \( J' \) generates averages of the spins with the indices involved and brings down a prefactor \( \beta \sqrt{1-t}/\sqrt{N} \) (for \( J \)) or \( \beta \sqrt{t} \sqrt{N} \) (for \( J' \)). Fortunately, two derivatives of \( \log Z_t \) are all we need because when equation (A.7) is evaluated, all terms containing higher-order derivatives drop out. This is left as an
exercise for the reader. Only the following terms survive:

\[ E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = \frac{\beta^4}{4N^2} \left( 2 - \frac{\sqrt{1-t^2}}{\sqrt{1-\tau^2}} - \frac{\sqrt{1-\tau^2}}{\sqrt{1-t^2}} \right) \]

\[ \times E \sum_{i<j,k<l} \left( \langle s_is_js_ksl \rangle_t - \langle s_is_j \rangle_t \langle s_ksl \rangle_t \right) \left( \langle s_is_js_ksl \rangle_\tau - \langle s_is_j \rangle_\tau \langle s_ksl \rangle_\tau \right) \]

\[ + \frac{\beta^2}{4N\sqrt{1-t^2}} \sum_{i<j} E \langle s_is_j \rangle_t \langle s_is_j \rangle_\tau \]

\[ + \frac{\beta^2}{4N\sqrt{1-\tau^2}} \sum_{i<j} E \langle s_is_j \rangle_t \langle s_is_j \rangle_\tau. \]  

(A.10)

In this equation, the last term is equal to the penultimate one due to symmetry under the exchange \( t \rightarrow 1-t \) and \( \tau \rightarrow 1-\tau \). In this equation, we can let the sums run unrestrictedly over \( i, j, k, l \) by introducing a factor of \( \frac{1}{4} \) for the first sum and a factor of \( \frac{1}{2} \) and a correction for the diagonal terms in the second sum, resulting in

\[ E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = \frac{\beta^4}{16N^2} \left( 2 - \frac{\sqrt{1-t^2}}{\sqrt{1-\tau^2}} - \frac{\sqrt{1-\tau^2}}{\sqrt{1-t^2}} \right) \]

\[ \times E \sum_{ijkl} \left( \langle s_is_js_ksl \rangle_t - \langle s_is_j \rangle_t \langle s_ksl \rangle_t \right) \left( \langle s_is_js_ksl \rangle_\tau - \langle s_is_j \rangle_\tau \langle s_ksl \rangle_\tau \right) \]

\[ + \frac{\beta^2}{4N\sqrt{1-t^2}} \left( \sum_{ij} E \langle s_is_j \rangle_t \langle s_is_j \rangle_\tau - N \right). \]  

(A.11)

We can write \( \sum_{ij} \langle s_is_j \rangle_t \langle s_is_j \rangle_\tau \) as \( N^2 \langle((1/N) \sum_i s_i^{t\tau} s_i^{3\tau})^2\rangle \), i.e. as a square of the spin overlap

\[ q_{13}(t, \tau) = \frac{1}{N} \sum_i s_i^{t\tau} s_i^{3\tau} \]  

(A.12)

between two replicas labelled 1 and 3 with different interpolation parameters \( t \) and \( \tau \). The labels 1 and 3 have been chosen because we will shortly need two more replicas which will be assigned the labels 2 and 4. Replicas 1 and 2 are then understood to have interpolation parameter \( t \) and replicas 3 and 4 to have the parameter \( \tau \). The angular brackets \( \langle \cdots \rangle \) without subscripts indicate the thermal average of a system comprising independent replicas with interpolation parameters \( t \) and \( \tau \).

A similar decomposition in replicas can be made in the first part of equation (A.11), but here two more replicas are needed. We find

\[ \frac{1}{N^4} \sum_{ijkl} \left( \langle s_is_js_ksl \rangle_t - \langle s_is_j \rangle_t \langle s_ksl \rangle_t \right) \left( \langle s_is_js_ksl \rangle_\tau - \langle s_is_j \rangle_\tau \langle s_ksl \rangle_\tau \right) \]

\[ = \frac{1}{N^4} \sum_{ijkl} \left( \langle s_i^{1\tau} s_j^{1\tau} s_k^{1\tau} s_l^{1\tau} \rangle - \langle s_i^{1\tau} s_j^{1\tau} \rangle \langle s_k s_l \rangle^{1\tau} \right) \left( \langle s_i^{3\tau} s_j^{3\tau} s_k^{3\tau} s_l^{3\tau} \rangle - \langle s_i^{3\tau} s_j^{3\tau} \rangle \langle s_k s_l \rangle^{3\tau} \right) \]

\[ - \langle s_i^{4\tau} s_j^{4\tau} \rangle \langle s_k^{3\tau} s_l^{3\tau} \rangle = \langle (q_{13}^2 - q_{14}^2)(q_{23}^2 - q_{24}^2) \rangle \]

\[ = \frac{1}{N^4} \left( \sum_{ij} \langle s_i^{1\tau} s_j^{1\tau} \rangle - \langle s_i^{1\tau} s_j^{1\tau} \rangle \langle s_i^{3\tau} s_j^{3\tau} \rangle \right)^2 \geq 0. \]  

(A.13)
As a by-product, we see in the last line that the expression $\langle (q_{i1}^2 - q_{i4}^2)(q_{i3}^2 - q_{23}^2) \rangle$ is nonnegative. The end result is finally

$$E \frac{\partial}{\partial t} \log Z_t \frac{\partial}{\partial \tau} \log Z_\tau = \frac{N^2 \beta^4}{16} \left( 2 - \frac{\sqrt{1 - \tau \sqrt{\tau}}}{\sqrt{1 - \tau \sqrt{\tau}}} - \frac{\sqrt{1 - \tau \sqrt{\tau}}}{\sqrt{1 - \tau \sqrt{\tau}}} \right) E \langle (q_{i1}^2 - q_{i4}^2)(q_{i3}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{4 \sqrt{\tau}} \left( E \langle q_{i1}^2 \rangle - \frac{1}{N} \right).$$

(A.14)

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