

Free-Energy Fluctuations and Chaos in the Sherrington-Kirkpatrick Model

T. Aspelmeier

Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen, Germany

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The sample-to-sample fluctuations ΔF_N of the free-energy in the Sherrington-Kirkpatrick model are shown rigorously to be related to bond chaos. Via this connection, the fluctuations become analytically accessible by replica methods. The replica calculation for bond chaos shows that the exponent μ governing the growth of the fluctuations with system size N , $\Delta F_N \sim N^\mu$, is bounded by $\mu \leq \frac{1}{4}$.

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The sample-to-sample fluctuations of the free-energy in the mean-field Ising spin glass [1] are a long standing unsolved problem in spin glass physics. In addition to their intrinsic interest as a finite-size effect in spin glasses, they are of fundamental importance for the physics of finite-dimensional spin glasses. It has been shown [2] that the finite-size scaling of the free-energy fluctuations ΔF_N in the mean-field spin glass is equal to the scaling of the domain wall energy ΔF_{DW} in finite dimensions $d \geq 6$, i.e. $N^\mu \propto \Delta F_N \propto \Delta F_{DW} \propto L^\theta$, where N is the total system size and L its linear dimension (in the case of a finite-dimensional system). This implies the relationship $\theta = d\mu$ between the domain wall exponent θ and the fluctuation exponent μ .

Chaos is also a very important aspect of spin glasses. Chaos refers to the property that an infinitesimal change of, for instance, the temperature or the bond strengths results in a complete change of the equilibrium state. Chaos was first suggested for hierarchical models and in the context of the droplet picture and finite-dimensional spin glasses [3,4] but has also been studied in mean-field models [5–7].

In this paper we derive a new and exact connection between the free-energy fluctuations and the seemingly unrelated phenomenon of chaos. Such a connection has been suggested by Bouchaud *et al.* [8] as part of a heuristic argument to obtain the free-energy fluctuations. Our results partly corroborate the argument but we will see that a crucial ingredient seems to be missing from it. In addition to making the heuristic argument precise, our results provide a new way to access the fluctuations analytically. The fluctuations are a subextensive quantity such that their calculation usually requires higher order terms in the loop expansion. These are, however, inaccessible due to the massless modes present throughout the spin glass phase. Here we will show that it is sufficient to calculate chaos to zero-loop order to obtain the fluctuations. We demonstrate this explicitly above and at the critical temperature but believe and present evidence that it also works in the low temperature phase.

The method we use to derive the connection between fluctuations and chaos is a variation of the interpolating Hamiltonian method, inspired by the work of Billoire [9] where a similar method was introduced to study the finite-

size corrections to the free energy numerically. In this Letter, we will set up a general formalism which will be amenable to an analytical treatment and derive the upper bound $\mu \leq \frac{1}{4}$. The details of the calculation will be published elsewhere [10].

Numerically, the sample-to-sample fluctuations in the mean-field model have been investigated extensively in the literature [2,11–15]. In all of these cases the study was restricted to zero temperature. The fluctuation exponent appears to be $\mu \approx 0.25$, although other values of μ can not entirely be ruled out. However, $\mu = \frac{1}{4}$ would violate the relation $\theta = d\mu$ since the numerical results for θ in high dimensions by Boettcher [16,17] give for instance $\theta = 1.1 \pm 0.1$ for $d=6$ while $d\mu = 1.5$ for $\mu = 0.25$. It is not entirely clear whether the exponent μ is the same at $T = 0$ and at finite temperature. While it most likely is identical, this is very hard to check since it is difficult to calculate μ numerically at any finite temperature. With the connection to chaos, however, it will be possible in the future to calculate μ at finite temperature by simulating chaos.

Other values than 0.25 for μ have been put forward in the literature. Crisanti *et al.* [18] found, using a result at zero-loop order by Kondor [19], that $\mu = \frac{1}{6}$. The argument is, however, not entirely rigorous. Nevertheless, it has recently been argued by a combination of heuristic arguments and extensive numerical simulations at finite temperature that $\mu = \frac{1}{6}$ is indeed correct [20]. The bound $\mu \leq \frac{1}{4}$ derived here is compatible with this but, unfortunately, does not rule out $\mu = \frac{1}{4}$.

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 , a Taylor expansion of $\log \overline{Z^n}$ in powers of n yields $\log \overline{Z^n} = -n\beta F_N + \frac{n^2}{2} \Delta F_N^2 + \dots$, where the overbar means the average over the disorder, $\beta = 1/k_B T$ is the inverse temperature and F_N is the average free energy at system size N . The dots indicate higher order cumulants. Using the standard replica formalism [21], one can calculate $\overline{Z^n}$ for integer n and try to continue the resulting expression to real n and isolate the coefficient of the second order term which represents the fluctuations. It is easy to show 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

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

[18,22]. A straightforward extension of the calculation in [22] shows that the fluctuations at the critical point are

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

Note that Eq. (1) is a one-loop result. Equation (2) even requires reorganization of the perturbation series [22]. We will see below that we can obtain precisely the same results from a zero-loop order calculation of bond chaos.

Interpolating Hamiltonians.—In order to derive the connection between the fluctuations and chaos, we introduce the following interpolating Hamiltonians:

$$\mathcal{H}_t^{(r)} = -\sqrt{\frac{1-t}{N}} \sum_{i < j} J_{ij} s_i s_j - \sqrt{\frac{t}{N}} \sum_{i < j} J_{ij}^{(r)} s_i s_j \quad (3)$$

with N Ising spins s_i , $0 \leq t \leq 1$, $r = 1, 2$ and J_{ij} , $J_{ij}^{(1)}$, $J_{ij}^{(2)}$ 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 Hamiltonians describe a normal spin

glass, the coupling constants being $\sqrt{1-t}J_{ij} + \sqrt{t}J_{ij}^{(r)}$ which are Gaussian random variables of unit variance.

The partition functions of these Hamiltonians are $Z_t^{(r)} = \text{Tr} \exp(-\beta \mathcal{H}_t^{(r)})$. Denoting the average over all coupling constants J_{ij} , $J_{ij}^{(1)}$ and $J_{ij}^{(2)}$ by E_J , it is straightforward to show that

$$E_J (\log Z_1^{(1)} - \log Z_0^{(1)})^2 = 2\beta^2 \Delta F_N^2, \quad (4)$$

$$E_J (\log Z_1^{(1)} - \log Z_0^{(1)}) (\log Z_1^{(2)} - \log Z_0^{(2)}) = \beta^2 \Delta F_N^2. \quad (5)$$

This gives us two distinct representations of the fluctuations. Using the idea from [23] to represent $\log Z_1^{(r)} - \log Z_0^{(r)}$ by differentiating with respect to the interpolation parameter and immediately integrating again, the fluctuations can be written in two ways as

$$\beta^2 \Delta F_N^2 = \frac{1}{2} \int_0^1 dt \int_0^1 d\tau E_J \frac{\partial \log Z_t^{(1)}}{\partial t} \frac{\partial \log Z_\tau^{(1)}}{\partial \tau}, \quad (6)$$

$$= \int_0^1 dt \int_0^1 d\tau E_J \frac{\partial \log Z_t^{(1)}}{\partial t} \frac{\partial \log Z_\tau^{(2)}}{\partial \tau}. \quad (7)$$

In [10] it will be shown how to manipulate this expression in order to arrive at the following Eqs. (8) and (9),

$$E_J \frac{\partial \log Z_t^{(1)}}{\partial t} \frac{\partial \log Z_\tau^{(1)}}{\partial \tau} = \frac{N^2 \beta^4}{16} h(t, \tau) E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{4\sqrt{t\tau}} \left(E_J \langle q_{13}^2 \rangle - \frac{1}{N} \right), \quad (8)$$

$$E_J \frac{\partial \log Z_t^{(1)}}{\partial t} \frac{\partial \log Z_\tau^{(2)}}{\partial \tau} = \frac{N^2 \beta^4}{16} E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{8\sqrt{1-t}\sqrt{1-\tau}} \left(E_J \langle q_{13}^2 \rangle - \frac{1}{N} \right), \quad (9)$$

with $h(t, \tau) = 2 - \frac{\sqrt{1-t}\sqrt{\tau}}{\sqrt{t}\sqrt{1-\tau}} - \frac{\sqrt{1-\tau}\sqrt{t}}{\sqrt{\tau}\sqrt{1-t}}$. Note that these equations are exact. The angular brackets $\langle \dots \rangle$ denote the thermal average and $q_{ab}(t, \tau) = \frac{1}{N} \sum_i s_i^{a,t} s_i^{b,\tau}$ are overlaps between independent replicas a, b with different interpolation parameters. The expression involving four replicas is always nonnegative, as can be seen from the following representation,

$$\begin{aligned} \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle &= \frac{1}{N^4} \sum_{ijkl} (\langle s_i^{1,t} s_j^{1,t} s_k^{1,t} s_l^{1,t} \rangle - \langle s_i^{1,t} s_j^{1,t} \rangle \langle s_k^{1,t} s_l^{1,t} \rangle) (\langle s_i^{3,\tau} s_j^{3,\tau} s_k^{3,\tau} s_l^{3,\tau} \rangle - \langle s_i^{3,\tau} s_j^{3,\tau} \rangle \langle s_k^{3,\tau} s_l^{3,\tau} \rangle) \\ &= \frac{1}{N^4} \left\langle \left(\sum_{ij} (s_i^{1,t} s_j^{1,t} - \langle s_i^{1,t} s_j^{1,t} \rangle) (s_i^{3,\tau} s_j^{3,\tau} - \langle s_i^{3,\tau} s_j^{3,\tau} \rangle) \right)^2 \right\rangle \geq 0. \end{aligned} \quad (10)$$

The last important step is to employ the fact that for any given value of t , $\mathcal{H}_t^{(r)}$ represents a normal mean-field spin glass with Gaussian couplings just like any other. Consider Eq. (8). The overlap q_{ab} between two replicas with different interpolation parameters is nothing but the overlap between two normal spin glasses with identical bonds (if $t = \tau$), uncorrelated bonds (if $t = 0$, $\tau = 1$ or vice versa) or correlated bonds (for anything in between). Similarly, for Eq. (9) the overlap is between systems with equal bonds ($t = \tau = 0$), totally uncorrelated bonds ($t = 1$ or $\tau = 1$) or correlated bonds (anything else). This shows the connection to bond chaos.

The overlaps in Eqs. (8) and (9) thus do not depend on t and τ separately but only on a measure of “distance” ϵ

between the two sets of bonds. We define ϵ via the correlation between the bonds, i.e., we set $\frac{1}{\sqrt{1+\epsilon^2}} = E_J (\sqrt{1-t}J_{ij} + \sqrt{t}J_{ij}^{(1)}) (\sqrt{1-\tau}J_{ij} + \sqrt{\tau}J_{ij}^{(1)}) = \sqrt{1-t}\sqrt{1-\tau} + \sqrt{t\tau}$ for Eq. (8) and $\frac{1}{\sqrt{1+\epsilon^2}} = E_J (\sqrt{1-t}J_{ij} + \sqrt{t}J_{ij}^{(1)}) (\sqrt{1-\tau}J_{ij} + \sqrt{\tau}J_{ij}^{(2)}) = \sqrt{1-t}\sqrt{1-\tau}$ for Eq. (9). With these definitions, $\epsilon = 0$ means identical bonds and $\epsilon = \infty$ means totally uncorrelated bonds.

We can now make a change of variables under the integrals in Eqs. (6) and (7) and eliminate, say, τ in favor of ϵ . The remaining integral over t can be carried out analytically and we get the two different exact expressions

$$\beta^2 \Delta F_N^2 = -\frac{N^2 \beta^4}{16} \int_0^\infty d\epsilon f_1(\epsilon) E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{4} \int_0^\infty d\epsilon g_1(\epsilon) \left(E_J \langle q_{13}^2 \rangle - \frac{1}{N} \right) \quad (11)$$

$$= +\frac{N^2 \beta^4}{16} \int_0^\infty d\epsilon f_2(\epsilon) E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle + \frac{N \beta^2}{4} \int_0^\infty d\epsilon g_2(\epsilon) \left(E_J \langle q_{13}^2 \rangle - \frac{1}{N} \right), \quad (12)$$

where

$$f_1(\epsilon) = \frac{4\epsilon^2 \arcsin \frac{1}{\sqrt{1+\epsilon^2}}}{(1+\epsilon^2)^2}, \quad g_1(\epsilon) = \frac{2 \arcsin \frac{1}{\sqrt{1+\epsilon^2}}}{(1+\epsilon^2)^{3/2}}, \quad (13)$$

$$f_2(\epsilon) = \frac{2\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^2}, \quad g_2(\epsilon) = \frac{\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^{3/2}}. \quad (14)$$

By going over from t and τ to ϵ the distinction between the different Hamiltonians in the two representations of the fluctuations has disappeared and the overlaps as a function of ϵ in both of these equations are the same.

Note the minus sign in front of the first term in Eq. (11) as opposed to the plus sign in Eq. (12). Since the function $f_1(\epsilon)$ is nonnegative and $\langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle \geq 0$, the first term is indeed a negative contribution. We conclude that the second term in Eq. (11) is an upper bound for the fluctuations.

Probability distribution of the overlap.—If we had the disorder averaged probability distribution $P_\epsilon(q)$ to find the overlap q between two replicas with bond distance ϵ , we could evaluate $E_J \langle q_{13}^2(\epsilon) \rangle$. In order to evaluate $E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle$ we need the probability distribution $P_\epsilon^{123}(q_{13}, q_{23})$ to simultaneously find q_{13} and q_{23} , as well as the probability distribution $P_\epsilon^{1234}(q_{14}, q_{23})$ to find q_{14} and q_{23} . However, in this Letter we will focus on $P_\epsilon(q)$.

The probability distribution $P_\epsilon(q)$ can be calculated approximately from large deviation statistics principles by considering two replicas with bonds J_{ij}^0 and $J_{ij}(\epsilon)$ which are a bond distance ϵ apart and constraining their overlap to a given value of q . The partition function $Z_{\epsilon,J}(q)$ of this combined system is

$$Z_{\epsilon,J}(q) = \text{Tr} \delta \left(q - \frac{\sum_i s_i t_i}{N} \right) \exp \left(\beta \sum_{i < j} (J_{ij}^0 s_i s_j + J_{ij}(\epsilon) t_i t_j) \right). \quad (15)$$

The variables s_i and t_i are the spin variables of the two replicas. From this one gets the average free energy per spin $\beta f_\epsilon(q) = -\frac{1}{N} E_J \log Z_{\epsilon,J}(q)$ and $P_\epsilon(q)$ is approximated by

$$P_\epsilon(q) \approx P_\epsilon^0(q) := \frac{e^{-N\beta f_\epsilon(q)}}{\int_0^1 dq e^{-N\beta f_\epsilon(q)}}. \quad (16)$$

Averages over $P_\epsilon^0(q)$ will be denoted by $[\dots]_0$.

A more precise discussion of the finite-size effects and the relevance for “small” deviations will be given in [10]. Here we will show that $P_\epsilon^0(q)$ is indeed the correct probability distribution to use by demonstrating that it yields the exactly known results above and at the critical temperature and by comparing predictions in the spin glass phase with simulations from [7] (see below).

Replica calculation.—To the best of our knowledge, bond chaos has never been calculated in the literature and we will therefore present a brief sketch of our results here. Since these replica calculations are fairly standard, we refer the reader to the analogous calculation for temperature chaos [5,6] for details. Repeating Rizzo’s calculation [5] for the constrained two-replica partition function from Eq. (15) but for bond chaos rather than temperature chaos, one arrives at the following truncated replica free energy

$$\beta f_\epsilon(q) = qp_d - \frac{p_d^2}{2} - \frac{yp_d^4}{6} - \frac{q^2}{2(1-2\tau')} + \tau \int_0^1 dz q^2(z) + \tau' \int_0^1 dz p^2(z) + \frac{y}{6} \int_0^1 dz [q^4(z) + p^4(z)] - \frac{w}{3} \int_0^1 dz z q^3(z) - w \int_0^1 dz z p^2(z) q(z) - w \int_0^1 dz \int_z^1 dz' [(q^2(z) + p^2(z))q(z') + 2p(z)q(z)p(z')] + 2wp_d \int_0^1 dz p(z)q(z). \quad (17)$$

The parameters w and y are equal to 1 for the SK model and $\tau = (\beta^2 - 1)/(2\beta^2)$ is the distance from the critical temperature $T_c = 1/\beta_c = 1$. The only reference to the bond distance is contained in $\tau' = (\beta^2 - \sqrt{1+\epsilon^2})/(2\beta^2)$. Three saddle point equations can be derived from this free energy by differentiating with respect to $q(x)$, $p(x)$ and p_d . The function $q(x)$ is the Parisi function for the overlap of the first replica with itself (the same function applies by symmetry to the overlap of the second replica with itself). The function $p(x)$ describes the overlap between replicas one and two. The parameter p_d stems from the diagonal of the overlap matrix between

replicas one and two and is a conjugate variable to the forced overlap q .

Solving the saddle point equations is nontrivial and only possible in certain limiting cases. Deferring the details to [10], we summarize the results here. Above the critical temperature we find $\beta f_\epsilon(q) = \frac{q^2}{2} (1 - \frac{\beta^2}{\sqrt{1+\epsilon^2}}) + \mathcal{O}(q^4)$. With this we can calculate $P_\epsilon^0(q)$ according to Eq. (16). Above the critical temperature, there is no replica symmetry breaking and the distributions $P_\epsilon^{123}(q_{13}, q_{23})$ and $P_\epsilon^{1234}(q_{13}, q_{24})$ factorize into a product of $P_\epsilon^0(q)$ ’s. The expression $E_J \langle (q_{13}^2 - q_{14}^2)(q_{13}^2 - q_{23}^2) \rangle$ can thus be written

as $[q^4]_0 - [q^2]_0^2$. The integrals in Eq. (12) can then be evaluated exactly giving precisely the result from Eq. (1).

Exactly at the critical temperature there is still no replica symmetry breaking and the factorization of P_ϵ^{123} and P_ϵ^{1234} applies as above. We obtain $P_\epsilon^0(q) \sim e^{-Nwq^3/6}$ for $\epsilon \ll N^{-1/6}$ and $P_\epsilon^0(q) \sim e^{-Nq^2\epsilon^2/4}$ for $N^{-1/6} \ll \epsilon \ll 1$. These limiting cases are enough to calculate the leading behavior of the integrals in Eq. (12) and we get the same as in Eq. (2).

Below the critical temperature, replica symmetry breaking does apply and we can not factorize P_ϵ^{123} and P_ϵ^{1234} . Although it has been shown in [24,25] how to break down these probability distributions, the results only apply for $\epsilon = 0$. We therefore concentrate on the second integral in Eq. (11) which is an upper bound for the fluctuations. We find four regimes,

$$P_\epsilon^0(q) \sim \begin{cases} 1 & \epsilon \ll N^{-1/2} \\ e^{-Nc_1q^3\epsilon^2} & N^{-1/2} \ll \epsilon \ll N^{-1/5} \\ e^{-Nc_2q^2\epsilon^2} & N^{-1/5} \ll \epsilon \ll 1 \\ e^{-Nq^2f(\epsilon)} & \text{otherwise} \end{cases}, \quad (18)$$

where $c_{1,2}$ are constants and $f(\epsilon)$ is an (unimportant) function. Using these results we can calculate the leading behavior of $\int_0^\infty d\epsilon g_1(\epsilon) E_J \langle q_{13}^2 \rangle$ and obtain for the dominant contribution to the integral

$$\frac{N\beta^2}{4} \int_0^{N^{-1/5}} d\epsilon g_1(\epsilon) [q^2]_0 = N^{1/2} \int_0^{N^{3/10}} dx \mathcal{F}(x) \sim N^{1/2}, \quad (19)$$

where $x = \epsilon\sqrt{N}$ is a scaling variable and $\mathcal{F}(x)$ is a scaling function with the properties $\mathcal{F}(x) \rightarrow \text{const}$ ($x \rightarrow 0$) and $\mathcal{F}(x) \sim x^{-4/3}$ ($x \rightarrow \infty$). This behavior of $\mathcal{F}(x)$ is perfectly consistent with the numerical results for $[q]_0$ presented in [7]. This is strong evidence that the finite-size corrections are indeed irrelevant even in the low temperature phase. (Note $x' = N\epsilon^2$ is used as a scaling variable in [7] and the scaling of $[q]_0$ is investigated instead of $[q^2]_0$ as we do here. This is, however, only a trivial difference.)

Since Eq. (19) is an upper bound for the fluctuations, it follows that $\mu \leq \frac{1}{4}$.

Discussion.—We have shown that there exists a deep and exact relation between the free-energy fluctuations and chaos in spin glasses, Eqs. (11) and (12). A similar connection has been suggested by Bouchaud *et al.* in a heuristic argument [8]. Briefly, the argument runs as follows. When the bonds are changed randomly by an amount of order $1/\sqrt{N}$, the ground state of the system changes and we get a new ground state energy. In order to obtain a truly independent new bond configuration, we must change the bonds by an amount of order 1; i.e., we obtain a sequence of $\sim\sqrt{N}$ level crossings. Each of these contributes a random amount of order 1 to the change in ground state energy such that the final energy differs by an amount of order $N^{1/4}$ from the original ground state energy, i.e. $\mu = \frac{1}{4}$.

This argument corresponds precisely to the second term in Eq. (11). From Eq. (18) we see that the overlap does not change appreciably until $\epsilon \approx N^{-1/2}$ (corresponding to the statement that the ground state does not change up to that value of ϵ), and the leading contribution to the fluctuations comes from tuning ϵ from 0 to $\mathcal{O}(1)$ and is proportional to $N^{1/4}$. There is, however, the negative first term in Eq. (11) which has no correspondence in the heuristic argument and which reduces the size of the fluctuations and might decrease μ . We are currently unable to provide an intuitive explanation for this term. We note, however, that it is crucial and cannot be ignored since in our second formulation, Eq. (12), the integral containing the four replica overlaps is the dominant term and is solely responsible for μ .

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