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Replica trick and fluctuations in disordered systems

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Abstract. — The finite volume fluctuations of the free energy in disordered systems can be characterized by means of the replica method. This is achieved by introducing a canonical ensemble in the space Ω of disorder realizations. In this space the role of energy is played by the free energy of the original system, and that of the temperature by n^{-1} , where n is the number of replicas. We apply this method to analyze the fluctuations in random directed polymers and in the Sherrington-Kirkpatrick model for spin glasses. Anomalous fluctuations are found in both cases. For the low temperature zero field phase of the Sherrington-Kirkpatrick model this approach predicts a $N^{-5/6}$ law for the relative fluctuations of the free energy per spin of a N-spin system.

The analysis of finite volume fluctuations in disordered systems is a subject which has attracted an increasing attention in recent times. One of the central issues is the comprehension of mesoscopic effects which can become quite relevant in many experimental situations. The replica method is one of the most important tools for the study of this problem [1].

As far as we know, the first result on this subject has been obtained by Toulouse and Derrida [2] who reconstruct the probability distribution of the free energy in the high temperature phase of the Sherrington-Kirkpatrick (SK) model [3] from the moments of the partition function, i.e., from the free energy per spin f(n) of n non-interacting replicas.

The aim of this paper is to show how the replica formalism can give informations on the finite size fluctuations of the free energy among different realizations of couplings in spin glasses and other disordered systems.

Consider a generic spin model with Hamiltonian:

$$H_N[\mathbf{J}] = -\sum_{i < j}^{1,N} J_{ij} \sigma_i \sigma_j - h \sum_{i}^{1,N} \sigma_i \tag{1}$$

where $\sigma_i = \pm 1$ is the value of the spin on the site i, the couplings J_{ij} are independent random variables with probability distribution $P[\mathbf{J}]$, and h is an external magnetic field.

For any fixed coupling realization **J**, the partition function of the N-spin system at temperature $1/\beta$ is given by

$$Z_N[\mathbf{J}] = \sum_{\{\sigma\}} \exp(-\beta H_N[\mathbf{J}]). \tag{2}$$

The quenched free energy per spin is $f_N = -\overline{\ln Z_N}/N\beta$, where $\overline{(\cdots)}$ indicates the average over the couplings realizations. We assume that the thermodynamic limit of the free energy, $-\lim_{N\to\infty} \ln Z_N[\mathbf{J}] / N\beta$ exists and is equal to the quenched free energy $f = \lim_{N\to\infty} f_N$ for almost all coupling realizations \mathbf{J} (self-average property). It is worth noting that this property corresponds in the context of dynamical systems, or of random matrix products, to the Oseledec theorem for the characteristic Lyapunov exponents [4]. Indeed if the partition function can be expressed with the help of transfer matrices, then f is the maximal Lyapunov exponent of the product of these matrices [5].

The analytic computation of the quenched free energy, i.e., of the average of the logarithm of the partition function, is a quite difficult problem, even in simple cases as nearest neighbour interaction in one dimensional models. However, since the integer moments of the partition function are easier computed, the standard method uses the so called "replica trick" by considering the annealed free energy $\mathcal{F}(n) = nf(n)$ of n non-interacting 'replicas' of the system [1],

$$\mathcal{F}(n) = -\lim_{N \to \infty} \frac{1}{N\beta} \ln \left[\overline{(Z_N[\overline{\mathbf{J}}])^n} \right]. \tag{3}$$

The quenched free energy of the original system is then recovered as the continuation of f(n) to n = 0,

$$f = -\lim_{n \to 0} \lim_{N \to \infty} \frac{\overline{(Z_N[\mathbf{J}])^n} - 1}{N\beta n} = \lim_{n \to 0} f(n).$$
 (4)

In real experiments or numerical simulations, the number of spins N is finite and the realization J fixed. Therefore what one computes is

$$y_N[\mathbf{J}] = -\frac{1}{N\beta} \ln Z_N[\mathbf{J}]. \tag{5}$$

The self-average property ensures that for almost all realizations $\mathbf{J} y_N \to f$ when $N \to \infty$. For large but finite systems y_N is still a random quantity whose probability distribution depends in a complicate way on that of \mathbf{J} . It is, therefore, important to study the (mesoscopic) fluctuations of the free energy (5) in large systems.

In general one may address two different questions. The first concerns the fluctuations of y_N about its average value $\overline{y_N}$ in a system of size N. Alternatively one may ask what are the deviations of y_N from the asymptotic value f.

To study the first question one can introduce the cumulant characteristic function as

$$\ln \overline{e^{-\beta Nyn}} = \ln \overline{Z_N^n} = \sum_{k=1}^{\infty} \frac{C_k}{k!} n^k$$
(6)

where C_k is the kth cumulant of $\ln Z_N$, i.e., $C_1 = \overline{\ln Z_N}$, $C_2 = \overline{(\ln Z_N)^2} - (\overline{\ln Z_N})^2$, etc. The factors β and N are introduced for convenience. From (3) and (7) we see that

$$\sum_{k=1}^{\infty} \frac{C_k}{k!} n^k = -\beta N \mathcal{F}_N(n) \tag{7}$$

where $\mathcal{F}_N(n)$ for integer and positive n is the free energy of n replicas on the system of size N. Thus if $\mathcal{F}_N(n)$ is known the cumulants are identified with the coefficients of the Taylor expansion of $\mathcal{F}_N(n)$ in powers of n. In particular the fluctuations of y_N about its average value are given by the coefficient of n^2 as

$$C_2 = \beta^2 N^2 \left(\overline{y_N^2} - \overline{y_N}^2 \right). \tag{8}$$

Unfortunately what one usually evaluates is not $\mathcal{F}_N(n)$ but its thermodynamic limit $\mathcal{F}(n)$ for $N \to \infty$. Consequently (7) has to be replaced by

$$-\beta \mathcal{F}(n) = \lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{\infty} \frac{C_k}{k!} n^k.$$
 (9)

From this equation it follows that if the cumulant C_k is o(N) then the term n^k will be missing in the Taylor expansion of $\mathcal{F}(n)$. In particular if, for example, $C_2 \sim N^{1-\gamma}$ with $\gamma > 0$ the expansion does not contain the n^2 term. Vice versa if this term is present, then

$$\overline{y_N^2} - \overline{y_N}^2 \sim N^{-1} \tag{10}$$

i.e. normal fluctuations. As a consequence the absence of the n^2 term in the expansion of $\mathcal{F}(n)$ signals anomalous fluctuations. In this case to have the correct scaling of C_2 with N one has to use $\mathcal{F}_N(n)$ which includes finite N corrections. In general, however, the calculation of $\mathcal{F}_N(n)$ is difficult, and hence the study of C_2 in presence of anomalous fluctuations is quite unpractical.

Informations on the deviations of y_N from its asymptotic value f, on the contrary, can be obtained directly from $\mathcal{F}(n)$ by using a method largely used in the last years to study the finite time fluctuations of the Lyapunov exponent in dynamical systems and of the localization length in the Anderson model [6].

The idea is to perform statistical mechanics in the space Ω of all the possible realizations of disorder **J**. For any fixed temperature β^{-1} , a state in this space corresponds to a well defined system with a given free energy y_N . The states in Ω can be classified according to the value y of y_N , and the space divided in classes $\omega(y)$ labelled by y. The probability distribution P(y) is hence proportional to the number of states in $\omega(y)$, i.e.,

$$P(y) \propto \left[\text{\# of states in } \omega(y) \right] \propto e^{-N S(y)}$$
 (11)

where by definition -N S(y) is the entropy of the class $\omega(y)$. We have explicitly displayed the extensive dependence on the system size N so that in the termodynamic limit $S(y) \sim O(1)$. We are indeed using a microcanonical ensemble in the Ω -space where the role of the energy is played by the free energy y of the original system. In particular, the self-average property of the free energy is equivalent to the existence of the thermodynamic limit in the Ω -space. As a consequence, -S(y) must be maximal for y=f. Since the entropy is defined a part from an additive constant, we can take S(y=f)=0 and S(y)>0 if $y\neq f$.

A direct calculation of S(y) is not easy, but from thermodynamics we know that it can be obtained from the free energy, which in the Ω -space reads

$$\int dy e^{-N(S(y)+\beta yn)} = e^{-N\beta n f(n)}$$
(12)

where $(\beta n)^{-1}$ is the temperature in the Ω -space. We have introduced the factor β for convenience. This does not change the results since we work at fixed temperature.

We are interested in the leading term of NS(y) in N, thus we can assume N very large in (12) and evaluate the integral by saddle point. This yields the usual relation between free energy and entropy

$$\beta n f(n) = \min_{y} \left[S(y) + \beta n y \right] \tag{13}$$

and the well known relation

$$\frac{\mathrm{d}S(y)}{\mathrm{d}y}\bigg|_{y^{\bullet}(n)} = -\beta n \tag{14}$$

among the entropy -S(y), the energy y and the temperature $(\beta n)^{-1}$ The relation (14) shows that each n selects a class $\omega(y^*)$ with free energy y^* . The higher n, the less probable is the corresponding class of realizations. We remark that in this way we consider only the extensive part of the entropy. In other words we neglect any term o(N) in the exponent of (11). In usual statistical mechanics terms o(N), in general, correspond to surface contributions. They do not affect the thermodynamic limit, but one should control their effects on the finite volume fluctuations. In generic systems, these terms are expected to be unimportant. We do not consider them on the same ground of what is done in the standard treatment of finite volume fluctuations in statistical mechanics. By this assumption, we can use (11) and (13) to derive some predictions on the finite volume behaviour of disordered systems.

The entropy can be obtained by inverting the Legendre transformation (13-14),

$$S(y) = \beta \mathcal{F}(n) - \beta ny \tag{15}$$

where n(y) has to be eliminated with respect to y with the help of

$$\frac{\mathrm{d}\mathcal{F}(n)}{\mathrm{d}n}\bigg|_{n(y)} = y \tag{16}$$

The important point is that to evaluate S(y) one needs just the extensive part of $\mathcal{F}(n)$ which, for integer positive n, is what one usually computes with the replica method.

Standard probability theory theorems [7] imply that f(n) is a monotonic, non increasing function of n. For small n we can expand $\mathcal{F}(n)$ in powers of n, i.e. an high temperature expansion in the Ω -space. Let us suppose that

$$\mathcal{F}(n) = fn - \frac{\mu}{2}n^2 + O(n^3). \tag{17}$$

with $\mu > 0$. Inserting this form into (15) and (16) one gets

$$S(y) = \beta \frac{(y-f)^2}{2\mu} \tag{18}$$

so that the variance of the fluctuations is given by,

$$\overline{(y-f)^2} = \frac{\mu}{N}.\tag{19}$$

In some cases it may happen that the n^2 term is missing. In this case (19) is not valid anymore. Assume for example that for n > 0

$$\mathcal{F}(n) = fn - \frac{a}{3}n^3 + O(n^4) \tag{20}$$

with a > 0 for convexity. Note that the condition $n \ge 0$ is necessary since (20) with a > 0 is not convex for n < 0. An easy calculation shows that this leads to,

$$S(y) = \frac{2}{3\sqrt{a}} (f - y)^{3/2} \quad \text{for } f - y \ge 0.$$
 (21)

The restriction on the sign of f-y follows from the restriction $n \ge 0$ in (20). This is similar to what one has in ordinary magnetic systems where an external field selects a phase of defined magnetization, e.g. positive or negative. Indeed, here n can be also seen as an external magnetic field, in which case y becomes a sort of magnetization. As for an ordinary magnetic field, the sign of n leads to a restriction on the sign of the magnetization, which in our case is f-y. In (21) we took $f-y \ge 0$ because S(y) was evaluated from $\mathcal{F}(n)$ with positive n, and hence in the n > 0 phase. Obviously S(y) so obtained gives informations on the probability distribution of y in the y < f phase.

Note that if the moments $\overline{Z^n}$ grows more than an exponential with n for $n \gg 1$ then the probability distribution is not uniquely determined by $\mathcal{F}(n)$ [8]. Nevertheless (21) gives informations on the small deviations from f. Therefore, from (21) we obtain that in the f-y>0 phase for large N

$$\overline{(f-y)} \propto N^{-2/3}, \qquad \overline{(f-y)^2} \propto N^{-4/3}$$

However, to calculate the cumulants, e.g. C_2 , we need the full probability distribution. Unfortunately we are not able to evaluate directly S(y) for y - f > 0 since this would require the calculation of $\overline{Z^n}$ for negative n.

By looking at (21) we see that the second derivative of S(y) with respect to y diverges as $y \to f^-$, i.e. $n \to 0^+$ This implies a second order phase transition in the Ω -space at n = 0. If we exclude some very patological cases, in general the critical exponents are equal from both sides of the critical point. By this assumption it readly follows that

$$S(y) = \frac{2}{3\sqrt{b}} (y - f)^{3/2} \qquad \text{for } y - f \ge 0.$$
 (22)

or, equivalently,

$$\mathcal{F}(n) = fn + \frac{b}{3}n^3 + O(n^4), \qquad n \le 0$$
 (23)

with b > 0. In general $a \neq b$.

A free energy of the form (20) appears in the study of random directed polymers [9]. In fact by employing a replica method one has for the integer positive moments of the partition function [9]

 $\overline{Z^n} = \exp\left[-f L(n-n^3)\right], \qquad L \gg 1 \tag{24}$

where L is the total length of the walk on the polymer. From the above result, therefore, one readily concludes that the probability distribution of the free energy F for small deviations from the asymptotic value Lf is

$$P(F) \propto \exp\left[-a_{\pm} |Lf - F|^{3/2} L^{-1/2}\right]$$
 (25)

where we take a_+ if Lf - F > 0 and a_- if Lf - F < 0. A similar form with $a_+ = a_-$ was proposed by Zhang [10], and later by Bouchaud and Orland [11]. However, in contrast with their formula, (25) leads, in general, to an asymmetric probability distribution. This is in agreement with recent numerical results [12].

From (25) one can conclude that if $a_{+} \neq a_{-}$

$$\overline{(Lf - F)} \propto L^{1/3} \tag{26}$$

in accord with references [10] and [11], and with the numerical results of Mézard [13]. By using (25) a straightforward calculation leads to the Kardar scaling [9]

$$C_2^{1/2} \sim L^{1/3} \tag{27}$$

Similarly one can find that $C_3^{1/3} \sim L^{1/3}$ The available numerical data [12] are in quite good accord with these scalings with the exponents 0.333 ± 0.003 for the second cumulant, and 0.37 ± 0.02 for the third.

The above arguments can be repeated for any powers of n, as long as there is a power n^m with m>1 in the expansion of the extensive part of $\mathcal{F}(n)-nf$. If the first non-vanishing power is n^m , then for m > 2

$$\frac{\overline{(f-y)}}{(f-y)^2} \propto N^{-(m-1)/m}$$
(28)

$$\overline{(f-y)^2} \propto N^{-2(m-1)/m} \tag{29}$$

Note that if $a_{+}=a_{-}$ then $\overline{(f-y)}=0$. In this case (28) is valid only if we restrict to the $f - y > 0 \ (< 0)$ phase.

As last example, we now apply this method to investigate the fluctuations in the Sherrington-Kirkpatrick (SK) model [3]. Before addressing the problem of the low temperature phase, let us spend a few words about the replica symmetric phase. In the high temperature phase, i.e., above the de Almeida and Thouless line there is no replica symmetry breaking [14]. An explicit calculation shows that for $h \neq 0$, the extensive part of $\mathcal{F}(n)$ contains the term n^2 [3]. On the other hand if h=0 the latter is missing and (19) is not valid. In this case $\mathcal{F}(n)=nf$, which can be seen formally as the $m \to \infty$ limit of the above case. Therefore from (28) and (29) it follows

$$\overline{(f-y)} \sim N^{-1}, \qquad \overline{(f-y)^2} \sim N^{-2} \tag{30}$$

Indeed an explicit calculation leads to [2]

$$\beta f = -\frac{\beta^2}{4} - \ln 2 - \frac{1}{4N} \ln(1 - \beta^2)$$

$$\beta \mu = -\frac{1}{2N} \left[\beta^2 + \ln(1 - \beta^2) \right]$$
(31)

where μ is the coefficient of the $n^2/2$ term, which can be related to $N(f-y)^2$. Note that μ diverges at the spin glass transition $\beta = 1$. This is a general result. The 1/N terms contain the fluctuations about the saddle point, and hence it is not difficult to understand that the coefficient of n^2/N should diverge at the spin glass transition where the replica symmetric solution becomes unstable [14].

The more interesting phase is, nevertheless, the low temperature phase where the replica symmetry is completely broken and many different minima of the free energy appear [1]. We limit ourselves to the case h=0. At the spin glass transition the overlap matrix $q_{\alpha\beta}$ between different replicas is zero and one may perform an expansion in powers of $q_{\alpha\beta}$. This leads to the so called "reduced" or "truncated" model. Using this model Kondor [15] found that the replica symmetric solution is stable only for $n > n_s = \frac{4}{3}\tau + \cdots$, where $\tau = (T_g - T)/T_g$ is the reduced temperature and T_g is the spin glass transition temperature. For $n < n_s$ a stable solution is found using the Parisi ansatz. This leads to [15]

$$f(n) = f_{\rm P}(\tau) - \frac{9}{5120} n^5 + \cdot$$
 for $n \le n_{\rm s}(\tau)$ (32)

with

$$f_{\rm P}(\tau) = \frac{\tau^3}{6} + \frac{\tau^4}{12} + \frac{\tau^5}{10}.\tag{33}$$

From (32) it follows that the first non-vanishing power (excluding the linear term) in the expansion of $\mathcal{F}(n)$ is n^6 and hence from (28) and (29) we have

$$\overline{(f-y)} \sim N^{-5/6}, \qquad \overline{(f-y)^2} \sim N^{-5/3}$$
 (34)

Assuming an asymmetric probability distribution, i.e. $a_{+} \neq a_{-}$, this result implies that the correction to the extensive part of the free energy is of order $N^{1/6}$, in agreement with recent suggestions [16]. A straigthforward calculation leads to the scaling law for the second cumulant

$$C_2 \sim N^{1/3} \tag{35}$$

Numerical data [17, 18] for the zero temperature energy fluctuations for systems of sizes $6 \le N \le 200$ leads to $C_2 \sim N^{\gamma}$ with $\gamma \simeq 1/2$. We note, however, that if only the data for $50 \le N \le 200$ are taken into account these can be fitted with $\gamma \simeq 1/3$ (see Fig. 9 Ref. [17]).

We conclude by noting that our arguments allows one to interpret the "searching for the maximum", which in the standard replica trick follows from the fact that the space dimensionality of the order parameter $q_{\alpha\beta}$ becomes negative for $n \to 0$, in a very natural way. In fact, the physics is given by the infinite temperature limit, in the Ω -space, and hence by the largest free energy. This also explains why in spin glasses the metastable states have lower free energies [19], which at first glance may look strange.

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