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SPIN GLASSES AND REPLICAS

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In this talk I present some of the basic ideas in the replica approach to the thermodynamics of spin glasses.

Much work has been devoted to spin glasses in recent years:[1] for reasons of time I will present only the approach based on the introduction of the replica symmetry and its spontaneous breaking. I think that it is very interesting for me to have the opportunity to present the replicas approach to vast audience of mathematical physicists; the method is very powerful but is impossible to follow the various steps of a computation using known mathematical techniques: very often you end up with a beautiful and deep result, but you do not understand how you obtained it, and it may take years to decipher the physical implications. A mathematical formalization of the approach would be a substantial leap forward.

At the present moment there are still some dark areas: I will not dare to present a logical approach starting from first principles, but I will rather follow an "historical" order.

A crucial role in this field has been played by the Sherrington Kirkpatrick[2] model (Ising model with infinite range random interaction): this model seems to be the simplest one containing some of the essential complications of more realistic models; it is believed that the comprehension of the S-K model would be a stepping stone in the field.

The Hamiltonian of the S-K model is the following:

$$H_{(N)}(J,\sigma) = \sum_{1}^{N-1}{}_i \sum_{i+1}^{N}{}_k J_{ik}\,\sigma_i\sigma_k - \sum_i h_i\,\sigma_i\,, \qquad (1)$$

where h is the external magnetic field, the σ_i are usual Ising spin variables (they can take values ±1) and the J_{ik} are independent randomly distributed variables with zero mean and variance 1/N. The probability distribution of the J_{ik} is thus:

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$$dP(j) = \prod_{1}^{N-1}{}_{i} \prod_{i+1}^{N}{}_{k} \left[\left(\frac{N}{2\pi}\right)^{\frac{1}{2}} \exp\left(\frac{-J_{ik}^2 N}{2}\right) d\, J_{ik} \right] . \quad (2)$$

For each choice of the J's we can define the partition function and the free energy density by using the canonical rules:

$$Z_N(J) = \sum_{\{\sigma\}} \exp[-\beta H_N\ (J,\sigma)]$$

$$F_N(J) = -\frac{1}{N\beta} \ell n\ [Z_N(J)] \quad (3)$$

We want to compute the average value of the free energy [with respect to the probability distribution (2)] in the thermodynamic limit:

$$\bar{F} \equiv \lim_{N\to\infty} F_N$$

$$\bar{F}_N \equiv \int dP(J)\ \ F_N(J) \quad (4)$$

(the bar will denote the average over the J's, the usual brackets (< >) the average over the σ's.)

It is believed (it is proved in the case of short range models)[3] that, for large N, $\bar{F}_N$ coincides with the most likely value of $F_N(J)$ i.e.

$$\lim_{N\to\infty} \overline{(F_N - \bar{F}_N)^2} \equiv \lim_{N\to\infty} \int dP(J)(F_N(J) - \bar{F}_N)^2 = 0\ , \quad (5)$$

in other words in the infinite volume limit all the choices of the J's leads to the same free energy density with probability one.

It is well known that the non-random analoque of the S-K model (all the J's equal to 1/N) can be solved exactly and the usual mean field theory gives the correct result if the limit N goes to infinity: in this case for constant magnetic field the partition function can be written as

$$Z_N = \left(\frac{N}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dm\ \exp\ [-N(\ \frac{m^2}{2} - \ell n\ ch(\beta m + \beta h))] \quad (6)$$

and in the large N limit the saddle point method can be used.

It is widely believed that the appropriate mean field theory for spin glasses should be strictly related to the exact solution of the S-K model and also that (in analogy with the deterministic case) the free energy of a spin glass with a short range interaction should be equal to the free energy of the

S-K model when the space dimensions become infinite; this last conjecture seems quite reasonable at least for hypertriangular lattices: H_N (eq. 1) can be regarded as the Hamiltonian of an elementary cell of an hypertriangular lattice in d dimensions (d=N-1).

The basic strategy for solving the S-K model consists in trying to use the saddle point method as in eq. 6: this can be done in the framework of the replica approach. The starting point are the following elementary identities:

$$\overline{F}_N = \lim_{n\to 0} F_N^{(n)}$$

$$F_N^{(n)} \equiv \frac{-1}{Nn\beta} \ln Z_N^{(n)}$$

$$Z_N^{(n)} \equiv \overline{(Z_N)^n} \equiv \int dP(J)(Z_N(J))^n \tag{7}$$

Now, for finite N, the $F_N^{(n)}$ are analytic functions of n, so, if the $F_N^{(n)}$ are known for integer positive n, it should be an unique (hoping for the best) analytic continuation in n. The replica method consists in finding compact expressions for integer n and to analytically continue the result. Indeed, for integer n, we obviously have:

$$Z^n(J) = \prod_{1}^{N}{}_a \, [Z(J)] = \prod_{1}^{n}{}_a \sum_{\{\sigma^a\}} \exp\,[-\,H(J,\sigma^a)]\,. \tag{8}$$

The integration over the J's can be now done (it is a Gaussian integral) and we end up with a partition function of a system of N x n Ising spins ($\sigma_i^a = \pm 1$). After some Gaussian integration we finally find (for simplicity at zero magnetic field):

$$Z_N^{(n)}(\beta) = Z_n^{(N)}\left(\left(\frac{n}{N}\right)^{\frac{1}{2}}\beta\right) =$$

$$= \int_{-\infty}^{+\infty} dQ\, \exp[-N\, A^{(n)}(Q)]$$

$$A^{(n)}(Q) = -\frac{\beta^2}{4} + \frac{1}{4}\sum_{1}^{n}{}_a \sum_{1}^{n}{}_b\, (\beta^2 Q_{ab}) +$$

$$\ln\{\sum_{\{S\}} \exp\,[\beta \sum_{1}^{n}{}_a \sum_{1}^{n}{}_b\, Q_{ab} S_a S_b]\}\,. \tag{9}$$

where Q_{ab} is a symmetric n x n matrix, identically zero on the diagonal ($Q_{aa} = 0\ \forall a$) and $S_a = \pm 1$.

In the limit N going to infinity the integral can be evaluated using the saddle point method; we obtain:

$$F^{(n)} \equiv -\frac{1}{\beta} \lim_{N\to\infty} F_N^{(n)} = -\frac{1}{\beta} \operatorname*{Min}_{Q} A^{(n)}(Q) \ . \qquad (10$$

Having solved the model for integer n we can now analytically continue the result up to n equal to zero.

In order to implement this program in an explicit way, the first task is to solve eq. 10: symmetry considerations are, as usual, quite useful. It is clear that the indices a and b label identical replicas of the same system: the function A(Q) must be invariant (as can be readily checked) under the action of the P_n group (the permutation group of n elements) acting simultaneously on the columns and on the rows of the matrix Q; more precisely if p_a is a permutation of n elements we have:

$$A(Q) = A(Q^P)$$

$$Q^P_{ab} = Q_{P_a P_b} \ . \qquad (11)$$

By general considerations we know that if a point is left invariant by the action of a symmetry group, it must be a stationary point of A(Q); an explicit computation is needed to check if it is the minimum. If the actual minimum is not left invariant by the action of the symmetry group (obviously all the points of the orbit must be a minimum) we normally say that the symmetry group is spontaneously broken.

Let us now see the consequences of the assumption (which will show up to be incorrect) that the group of permutation of replicas (the replica symmetry) is not broken. It is easy to see that the matrix Q must have the form:

$$Q_{ab} = q \quad \text{for } a \neq b \ . \qquad (12)$$

For this choice of Q it is easy to evaluate A(Q) for any n: the saddle point condition ($\frac{\partial A}{\partial A_{ab}} = 0$) becomes at n = 0:

$$q = \int_{-\infty}^{\infty} \frac{dz}{(2\pi)^{\frac{1}{2}}} \{\exp(-z^2/2)\ \mathrm{th}^2\ (\beta q^{\frac{1}{2}} z)\}. \qquad (13)$$

At high temperature eq. 13 has only the trivial solution q = 0; at T less than 1 a new solution appears with $q(T) \neq 0$:

$$q(T) \sim 1 - T \qquad T \sim 1$$

$$q(T) \sim 1 - T\sqrt{\pi} \qquad T \sim 0 \tag{14}$$

At the point T=1 the free energy is slightly singular: the temperature derivative of the specific heat is discontinuous. By adding an external magnetic field the transition disappears and q becomes different from zero in the whole temperature range. At this stage the physical interpretation of q is quite clear:[(4)] we easily find:

$$q = q_{EA} \equiv \overline{m_i^2} \equiv \overline{<\sigma_i>^2} \equiv \int dP[J] \; <\sigma_i>_J^2 \quad , \tag{15}$$

where the magnetization has been computed in an infinitesimal small magnetic field. It is important to realize that the probability distribution of the J's and the Hamiltonian (1) are both invariant at zero magnetic field under the "gauge" transformation:[5]

$$\sigma_i \rightarrow -\sigma_i \qquad J_{iK} \rightarrow -J_{iK} \qquad \forall\; K \; . \tag{16}$$

The free energy in presence of a constant magnetic field will be the same as in presence of a random magnetic field (provided that it is not correlated to the J's) and all quantities which are not invariant under (16) have a zero expectation value. The quantity q_{EA} is a good order parameter for the spin glass transition at h = 0: in the high temperature phase the magnetization is zero, while in the low temperature phase, as soon as $m_i \neq 0$, q_{EA} becomes different from zero. Usual arguments suggest that with probability one:

$$q_{EA} = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} <\sigma_i>_J^2 \quad . \tag{17}$$

If the solution here presented would be correct, spin glass would be very similar to an ordinary antiferromagnet, the direction in which the spontaneous magnetization points being random (and therefore having a projection of $O(N^{\frac{1}{2}})$ in the direction of a constant magnetic field). However it was realized from the beginning that the solution cannot be correct because it leads to a negative entropy in the low temperature region for all values of the magnetic field.[2,6]

Something wrong has been done. The fault has been found by De Almeida and

Thouless:[6] they observed that in order to apply the saddle point method it is absolutely necessary that the Hessian matrix

$$H_{ab;cd} = \frac{\partial^2 A}{\partial Q_{ab}\,\partial Q_{cd}} \tag{18}$$

has no negative eigenvalue at the saddle point. An explicit computation shows that this condition is not satisfied for

$$|h| < h_c(T)$$

$$h_c(T) \underset{T\to 0}{\to} \infty \qquad h_c(T) \sim (1-T)^{2/3}, \quad T \sim 1. \tag{19}$$

The previous solution is therefore wrong in the whole region $T < 1$, $h = 0$. Therefore in the low temperature region the saddle point cannot be replica-symmetric and the replica symmetry must be broken. A new solution of the saddle point equation must be found.

At this stage we are lost. An explicit computation[7] shows that the replica symmetry is restored for $n > n_c$ so that a phase transition in n is present and $F^{(0)}$ cannot be the analytic continuation of $F^{(n)}$; as usual the absolute minimum of a function which depends analytically on a parameter is only a local piecewise analytic function. The only way out consists in giving some meaning to $A^{(n)}(Q)$ also to non integer n, which more or less corresponds to defining an n x n matrix, when n is non integer. More precisley our task is to define P_n invariant functionals over the space of n x n matrices.

We proceed in the following way:[1] for any n, there is a finite list of algebraically independent P_n symmetric functions e.g.:

$$\mathrm{tr}(Q^K)\ ,\ \mathrm{tr}(Q{*}^K)\ ,\quad \mathrm{tr}(Q^{K_1}\cdot Q{*}^{K_2}\cdot Q^{K_3}),$$

$$\mathrm{Pr}(Q^K)\ ,\ \mathrm{Pr}(Q{*}^{K_1}\cdot Q^{K_2})\ ,\ \text{etc.} \tag{20}$$

where

$$(Q{*}^K)_{ab} = (Q_{ab})^K;\ \mathrm{tr}(R) = \frac{1}{n}\sum_a R_{a,a}\ ;\ \mathrm{Pr}(R) = \frac{1}{n(n-1)}\sum_1^n{}_a \sum_1^a{}_b\ {}_{a\neq b}\ R_{ab} \tag{21}$$

We say now that a given family of matrices $Q^{(n)}$ (each for every n) depends polynomially on n iff each of the invariants of the list is a polynomial in n. The space of n x n matrices is defined as the appropriate closure of the space of polynomial matrices. The final recipe is:

$$F^{(0)} = -\frac{1}{\beta} \operatorname*{Min}_{Q} A^{(0)} (Q) \tag{22}$$

where the minimum is taken over all the possible n x n matrices (according to the previous definition), such that:

$$\frac{\partial A}{\partial Q_{ab}} = 0 \tag{23}$$

the Hessian having no negative eigenvalue.

The correctness of this prescription is very unclear; moreover the evaluation of the r.h.s. of eq. (22) is very difficult: the space of n x n matrices is extremely large (it is certainly infinitely dimensional). The only positive result (up to now) is the construction of a solution of equation (23)[8] such that the corresponding Hessian has nonnegative eigenvalues;[9] (a second solution has been found,[10] however all the invariant functionals seem to have the same value, so it is unclear in which sense it is a different solution;[11] anyhow both solutions give the same free energy).

The explicit construction of the matrix Q which is a possible solution of eqs. 22 and 23 is rather involved and can be found in the literature;[8] we only recall that the matrix Q is a functional of a function Q(x) defined on the interval 0-1. One finds

$$\Pr(Q^{*K}) = \int_0^1 dx (Q(x))^K , \tag{24}$$

while other invariants have a slightly more complex form.

The function A(Q) is now a functional of Q(x): after some computations one finds:[8]

$$- F = \max_{Q(x)} A[Q]$$

$$A[Q] = -\frac{1}{4} \beta^2 \{1 + \int_0^1 Q^2(x)\, dx + 2Q(1)\} - a[Q], \quad a[Q] = f(o,h) \tag{25}$$

where the function f(x,y) satisfies the following differential equation:

$$\frac{\partial f}{\partial x} = -\frac{1}{2} \frac{dQ}{dx} \left[-\frac{\partial^2 f}{\partial y^2} + x \left(\frac{\partial f}{\partial y} \right)^2 \right] \tag{26}$$

with the boundary condition:

$$f(1,y) = \ell n[2ch\ (\beta y)] \ . \tag{27}$$

Eq. 27 is correct only if $Q(0) = 0$, otherwise:

$$a[Q] = \int_{-\infty}^{+\infty} \frac{dz}{(2\pi)^{\frac{1}{2}}}\ \exp\ (-z^{2}/2)\ f(0,\ h + \sqrt{Q(0)}z) \ . \tag{28}$$

The solution of these equations can be found analytically only for T near $T_c = 1$, numerical techniques must be applied elsewhere. The function $Q(x)$ is constant above the de Almeida Thouless line, otherwise it is a monotonous increasing function whose main features are:

$$\begin{aligned} &Q(x) = Q_m \quad \text{if } x < x_m, \quad Q(x) = Q_M \quad \text{if } x > x_M \\ &x_m \sim h^{2/3} \qquad Q_m \sim h^{2/3} \qquad x_m \sim (1-T) \\ &x_M - x_m \sim (h_c - h) \quad Q_M - Q_m \sim (h_c - h) \ . \end{aligned} \tag{29}$$

No negative eigenvalues of the Hessian are present (atleast for T near T_c) although there is an infinite number of eigenvalues accumulating near zero.[9] The numerical solutions strongly indicate that the zero temperature entropy is zero. The various thermodynamical quantities come out to be in remarkable good agreement with the Monte Carlo simulations. It is quite possible that eqs. 25-28 are the exact solution of the S-K model, indeed the same equations have been found using different arguments based on the time evolution of the system.[12] (There is a very interesting reformulation of these equations as stochastic differential equation).[1,13]

If we suppose to be on the right track, we face two problems: to give a physical interpretation to the breaking of the replica symmetry and to the order parameter $q(x)$. Quite recently a complete picture has been proposed based on the coexistence of different equlibrium states: we present here the main results.[14,15]

We recall that in statistical mechanics pure states (i.e. different phases) play a crucial role;[16] it is generally true that in the infinite volume limit the usual Gibbs states $<\ >$ may be decomposed into pure states (labeled by S):

$$<\ > \ = \Sigma_S\ W_S\ <\ >_S \tag{30}$$

W_S being the appropriate weights (for simplicity of writing we assume that the number of pure states is numerable and that $\Sigma W_S = 1$). In many models at non zero magnetic field there is only one pure state (the Gibbs state being consequently pure); this should happen also for spin glasses in the replica symmetric phase. It turns out that in the region where replica symmetry is broken many equilibrium states are possible also in presence of a constant magentic field; in this case the magnetization $m_i^{(S)} \equiv \langle\sigma_i\rangle_S$ will change from state to state:

$$\langle\sigma_i\rangle_S \neq \langle\sigma_i\rangle_{S'} \quad \text{if} \quad S \neq S' . \tag{31}$$

In each phase we can define an order parameter:

$$q_S = \lim_{N\to\infty} \frac{1}{N} \sum_1^N {}_i \langle\sigma_i\rangle_S^2 , \tag{32}$$

which is likely to be independent from the state, i.e. $q_S = q_S' \equiv q_{EA}$. It is certainly interesting to know how much different states differ one from the other; at this end we introduce the overlap of two states:

$$q_{SS'} = \lim_{N\to\infty} \frac{1}{N} \sum_1^N {}_v \langle\sigma_i\rangle_S \langle\sigma_i\rangle_{S'} \tag{33}$$

Obviously

$$q_{SS} = q_S . \tag{34}$$

It is useful to consider the probability distribution of averaged over the J's:

$$dP(q) = \sum_{S,S'} W_S W_{S'} \delta(q - q_{SS'}) \, dq , \tag{35}$$

We can also introduce the inverse function of P(q), q(x) which is defined on the interval 0 - 1:

$$\int_0^1 dx \quad q(x)^K = \int dP(q) \, q^K \quad \forall K \tag{35}$$

The function q(x) carries many informations on the relative orientation of different states; (if q(x) is a constant, essentially only one equilibrium state is present) the maximum value of $q(x)$ (i.e. $q(1)$ because the function $q(x)$ is monotonous by construction) can be identified with q_{EA}, while $q(0)$ is the minimum overlap among two different states; $\int dx\, q(x)$ must be identified with the square of the magnetization computed in the Gibbs state.

The interpretation of the breaking of the replica symmetry follows a simple argument which tells us that the two functions $Q(x)$ and $q(x)$ must be identified:

$$Q(x) = q(x) \ . \tag{37}$$

Recent numerical simulations support eq. (37).[17]

We have now in our hands a precise definition of the order parameter $Q(x)$ of the broken replica theory: it is rather remarkable that it took nearly fo years of thinking from going from eqs. (25-28) to eq. 37. When in 1979 I introduced the function $Q(x)$ and derived eqs. (25-28) I was led mainly by selfconsistency requirements which were internal to the formalism of broken replicas: the physical interpretation came only much later.

The richness in pure states of the S-K model is also displayed by the fol lowing phenomenon: let us define by $\bar{q}(\delta)$ the overlap between two Gibbs state which differ one from the other one by the addition of a small constant megnetic field in the Hamiltonian equal to $\delta/N^{\frac{1}{2}}$:

$$\bar{q}(\delta) = \lim_{N\to\infty} \frac{1}{N} \sum_{1}^{N}{}_{i} \langle\sigma_i\rangle_h \langle\sigma_i\rangle_{h+\delta/N^{\frac{1}{2}}} \tag{38}$$

Now it can be shown that $q(\delta)$ is a non trivial function of δ such that:

$$\lim_{\delta\to\infty} \bar{q}(\delta) = q(0) \qquad \bar{q}(0) = \int_0^1 dx\, q(x) \tag{39}$$

In other words when one changes the external magentic field of a factor is large with respect to $N^{-\frac{1}{2}}$, the set of states of the system changes comp and they have an overlap given by $q(0)$ which is the square of the persisten part of the spontaneous magnetization. Therefore with the change the magne field the system is automatically led to a metastable state and it may take a long time to return to a stable state; the existence of these first order microtransitions[19] (which form a dense set in the infinite volume limit) is at the origin of hysteresis (remanence) in the magnetic field.

The magnetic susceptibility will thus receive two contributions: the fir is the usual one and can be computed by using the linear response theory ir a given pure state (i.e. the reversible susceptibility χ_r), the second one comes from the jumping of the system from one state to another one χ_i (irreversible susceptibility)the total susceptibility χ_T (which can be computed by applying the linear response theory in the Gibbs state) will be the sum of the two; for small magnetic fields one finds:

$$\chi_r = \beta(1 - q(1)) \ , \quad \chi_T = \beta\int_0^1 dx \ (1 - q(x)), \ \chi_i = \beta\int_0^1 dx(q(1) - q(x)). \quad (40)$$

We could say that the signal of the breaking of the replica symmetry is the failure of the linear response theory for the susceptibility (i.e. $N\chi = \langle M - \langle M\rangle\rangle^2$, $M = \sum_1^N{}_i \sigma_i$) if the expectation values are taken in a pure state.

We see that the formalism of broken replica symmetry, originated to study random systems, contains many ideas which may be applied also to other non random systems with non random Hamiltonian, provided that the decomposition of the Gibbs state in pure states is non trivial; it would be rather interesting to implement this program for real glasses or for Ruelle's turbulent crystal.[20]

For finite dimensions short range interaction spin glasses the situation is not prefectly clear; in principle we could write an effective Hamiltonian (a la Landau Ginsburg) in replica space:

$$H(Q) = \int d^D x \ [\ \frac{1}{2} \text{Tr} \ (\partial_\mu \ Q)^2 + \frac{1}{2} m^2 \ \text{Tr} \ Q^2 + \ \frac{h^2}{2} \ \text{Tr} \ Q$$

$$+ \ g_3 \ \text{Tr} \ Q^3 + g_4 \ \ h \ Q\star^4 + \ldots] \quad (41)$$

and by using the standard technologies (perburbation theory, Goldstone bosons, renormalization group, non linear effective sigma model, etc..) it should be simple to find the critical exponents and the lower critical dimension, i.e. the smallest dimension for which a transition is present. Unfortunately there are serious technical difficulties in the first step, i.e. the construction of perturbation theory in the broken phase region: the resolvent of the Hessian is not easy to construct although some progress has been made recently.[9]

I hope to have convinced the audience of the usefulness of the replica - broken replica symmetry approach to spin glasses although the deep reasons of this success are still unclear.

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