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Replica Field Theory for Deterministic Models (II): A Non-Random Spin Glass with Glassy Behavior

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where the expectation value is defined by

$$\langle A(x) \rangle = \frac{\int dx \frac{e^{-x^2}}{\sqrt{2\pi}} \cosh^m(\sqrt{2\lambda}x) A(x)}{\int dx \frac{e^{-x^2}}{\sqrt{2\pi}} \cosh^m(\sqrt{2\lambda}x)}. \quad (62)$$

Inserting in (56) this value of μ we have searched among the 5 values of g the one which gives the maximum free energy when the stability is marginal (i.e. when (56) is saturated). We have found that the eigenvalue g_5 is the one which gives the maximal free energy. This leads us to the marginality condition (46). We have searched for a solution of the marginality condition in which m behaves linearly with T for low temperatures, but we have not been able to find it. It is plausible that such well behaved solution does not exist and that to improve our solution one would need to break the replica symmetry with a larger number of steps.

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$$\begin{aligned}
I_{(ab)(cd)} &= \frac{\partial^2 A}{\partial \Lambda_{ab} \partial Q_{cd}} = \delta_{(ab)(cd)} \\
M_{(ab)(cd)} &= \frac{\partial^2 A}{\partial \Lambda_{ab} \partial \Lambda_{cd}} = \langle \sigma_a \sigma_b \rangle_F \langle \sigma_c \sigma_d \rangle_F - \langle \sigma_a \sigma_b \sigma_c \sigma_d \rangle_F .
\end{aligned} \tag{55}$$

The mean value $\langle \dots \rangle_F$ in the last equations is taken over the action (39). M is the usual Hessian which determines the stability of the SK model.

Now it is easy to see that for each eigenvalue of the sub-block matrices G and M , (for instance g and μ respectively) the stability condition is determined by

$$g\mu - 1 \leq 0 , \tag{56}$$

the marginal condition being the equality. We have now to compute all the eigenvalues of the matrices G and M and to search for the ones which maximize the product $g\mu$. For the p -spin model (and also the SK model) this condition is relatively easy to determine because there is a unique eigenvalue g for G (in that case the matrix G is g times the identity matrix) and the maximum eigenvalue of M is found in the replicon sector when all replicas belong to the same block (once replica symmetry is broken).

In the present case even though the maximum value of M is the usual one [22] G has more than one eigenvalue. We have searched for all of them in case of one step of replica symmetry breaking. We have evaluated the derivatives for the matrices Q and Λ broken according to the scheme of (43). The general expression for the eigenvalues at one step of replica symmetry breaking has been given in [23]. There are two longitudinal eigenvalues, four anomalous eigenvalues and four replicons which finally reduce to only five different eigenvalues (this is because we set $Q_{(ab)} = 0$ if the indices (a, b) do not belong to the same sub-block of size m). These are given by

$$\begin{aligned}
g_1 &= \frac{16\beta^2}{m} (G''(4\beta(1-q)) + (m-1)G''(4\beta(mq+1-q))) \\
g_2 &= 16\beta^2 G''(4\beta(1-q+mq))
\end{aligned} \tag{57}$$

$$g_3 = \frac{32\beta^2}{m} G''(4\beta(1-q)) + \frac{4\beta(m-2)}{qm^2} (G'(4\beta(1-q+mq)) - G'(4\beta(1-q))) \tag{58}$$

$$g_4 = \frac{4\beta}{qm} (G'(4\beta(1-q+mq)) - G'(4\beta(1-q))) \tag{59}$$

$$g_5 = 16\beta^2 G''(4\beta(1-q)) . \tag{60}$$

g_5 is the replicon, where all the replica indices belong to the same sub-block. Taking for the matrix M the replicon eigenvalue corresponding to the four replica indices all belonging to the same sub-block we find

$$\mu = \langle \cosh^{-4}(\sqrt{2\lambda}x) \rangle , \tag{61}$$

Appendix

In this appendix we present some technical details about how we applied the marginality condition in our computation at one step of replica symmetry breaking. Our starting point is the expression for the free energy

$$A[Q, \Lambda] = -\frac{1}{2} \text{Tr}G(2\beta Q) + \text{Tr}(\Lambda Q) - F(\Lambda) , \quad (50)$$

with $G(Q)$ given by

$$G(2\beta Q) = \sum_{k \geq 1} \frac{(2\beta)^{2k}}{2k} \psi_{2k} \text{TrTr}Q^{2k} = \sum_{k \geq 1} c_{2k} \text{Tr}Q^{2k} , \quad (51)$$

where the ψ_{2k} are the Taylor coefficients of the series expansion of the function $\psi(z)$:

$$\psi(z) = 1 + \sum_{k \geq 1} \psi_{2k} z^{2k} . \quad (52)$$

In the most general case the stability condition implies that the Hessian matrix of the second derivatives of $A[Q, \Lambda]$ in the space of matrices $\{Q, \Lambda\}$ around the equilibrium solution is negative definite (the integration path in Λ space runs on is the imaginary axis, and the stability condition has the opposite sign than in the usual case). To construct the Hessian we compute the second derivatives of (50). This gives a four blocks matrix with the derivatives $\partial_{QQ}A$, $\partial_{\Lambda\Lambda}A$, $\partial_{Q\Lambda}A$ and the identical symmetric block $\partial_{\Lambda Q}A$. The sub-block $G \equiv \partial_{QQ}A$ is given by

$$G_{(ab)(cd)} = \frac{\partial^2 A}{\partial Q_{ab} \partial Q_{cd}} = \sum_{k \geq 1} 4k c_{2k} \frac{\partial(Q^{2k-1})_{ab}}{\partial Q_{cd}} . \quad (53)$$

The matrix G has three different types of elements, depending on if the replica indices (ab) and (cd) do coincide, have one element in common or are completely different. For these three different cases we have

$$\begin{aligned} \frac{\partial(Q^{2k-1})_{ab}}{\partial Q_{cd}} &= \sum_{p=0}^{2k-2} \left((Q^p)_{ac} (Q^{2k-2-p})_{db} + (Q^p)_{ad} (Q^{2k-2-p})_{cb} \right) \\ \frac{\partial(Q^{2k-1})_{ab}}{\partial Q_{ac}} &= \sum_{p=0}^{2k-2} \left((Q^p)_{aa} (Q^{2k-2-p})_{cb} + (Q^p)_{ac} (Q^{2k-2-p})_{ab} \right) \\ \frac{\partial(Q^{2k-1})_{ab}}{\partial Q_{ab}} &= \sum_{p=0}^{2k-2} \left((Q^p)_{aa} (Q^{2k-2-p})_{bb} + (Q^p)_{ab} (Q^{2k-2-p})_{ab} \right) . \end{aligned} \quad (54)$$

The other sub-blocks I and M are

prime values of $(2N + 1)$ the deterministic model admits a ground state based on Legendre sequences which we cannot find in the random approach) we have found that in all the metastable phase th two class of models coincide. We have also found, remarkably, that for generic values of N even the ground states of the models seem to coincide (as from figure (9)).

We have shown that for the values of N which satisfy the cardinality condition the deterministic model undergoes a crystallization transition. This transition is of the first order from the thermodynamical point of view, since the energy and the entropy jump discontinuously. Even if we cannot be sure of this fact, our exact solutions of small systems give a precise hint favoring the absence of a zero energy ground state for generic N values.

We have shown that the structure of metastable states of the two classes of models has much in common (at this effect the cardinality of N is irrelevant). For the model with quenched disorder we have performed Monte Carlo runs at zero temperature searching for locally stable states. In the deterministic case we have solved the naive TAP equations. The similarity of the shapes of the distribution of metastable states suggests that the dynamical behavior of the two models must be very similar. The two figures (11), (12) are quite decisive in this respect. The two models behave very similarly, they both display a singularity at a temperature T_G where the system freezes and thermodynamic fluctuations (related for example to the specific heat and to the magnetic susceptibility) vanish. We have also shown that for reasons that are quite unclear to us the marginality condition gives a good estimate of the low T behavior.

These results strengthen the idea that the off-equilibrium dynamics for the deterministic model should be very similar to the one of the model with quenched disorder. We would expect, for example, that the deterministic model could display aging effects like those which affect the random model and many models based on quenched disorder [21]. We have measured the usual time-time correlation function between the spin configuration at the waiting time t_w and the spin configuration at a later time $t_w + t$. We have observed that below T_G the shape of the correlation function depends on the previous history, i.e. on t_w . These results are much similar to those found also in related deterministic models like the low autocorrelation binary sequences [4]. It seems that also deterministic models display non-equilibrium effects very similar to those of spin glasses with randomness.

We hope that the results of this paper can be relevant to a large variety of different problems in condensed matter physics, where it is natural to study systems with a complex free energy landscape in which quenched disorder is not present as a given, preassigned condition.

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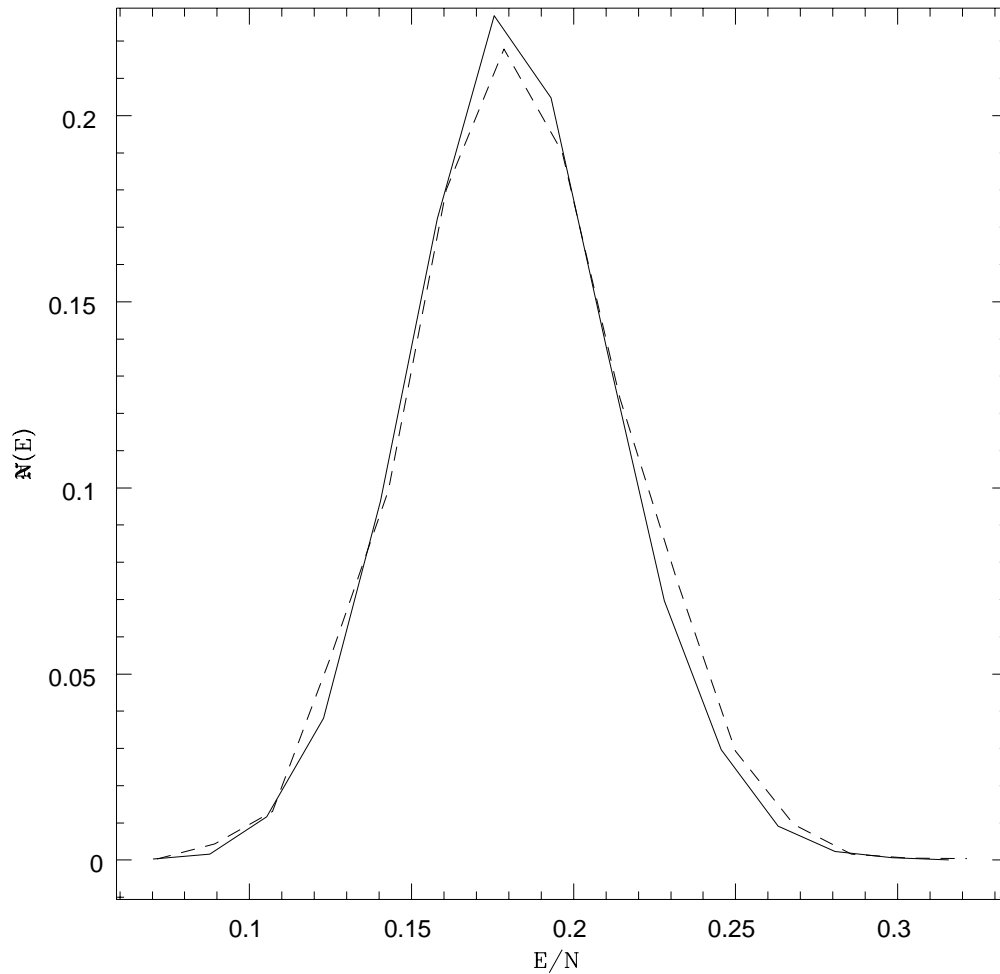


Figure 13: The number of solutions of the $T = 0$ mean field equations of a given energy as function of the energy for $N = 56$, where $(2N + 1)$ is prime (dashed line) and for $N = 57$, where $(2N + 1)$ is not prime (continuous line).

9 Mean Field Equations for the Deterministic Model

The naive mean field equations for the sine model can be defined through the iterative relation

$$m_x = \tanh\left(\beta \sum_{y \neq x} S_x(m_y)\right), \quad (48)$$

where the function S_x has been defined in (2). Obviously we could have defined the analogous equations by using the C function defined in eq. (4).

We are interested in the low temperature limit of the model. We can thus avoid to consider the complete TAP equations, where the reaction field is included, which are far more difficult to deal with. In the low temperature limit we can solve the even simpler equations

$$m_x = \text{sign}(h_x), \quad (49)$$

where h_x is the local field acting on the spin x .

We find the $T = 0$ solution of these equation by cooling the solution found at $T > 0$. In figure (13) we show the number of solutions of a given energy as function of the energy respectively for a typical prime (dashed line) and non prime value (continuous line) of $p = (2N + 1)$.

Analogously to (\mathcal{A}) we stop our ground state search after finding 5 times the states with the lowest energies. That makes us confident we have sampled the low energy states with good accuracy. We have studied systems with N up to 64. For prime values of $(2N + 1)$, where we know the exact ground state, this method has always found the correct ground state energy (i.e. zero).

10 Conclusions

Building upon the idea introduced in our former paper (\mathcal{A}) we have introduced here a class of deterministic spin models which do not contain disorder, but whose low T behavior is dictated by self-induced frustration. They are potentially relevant to the description of the glass state. Using number theory we have been able to exhibit a zero energy ground state for given values of the volume N (such that $(2N + 1)$ is prime).

We have proceeded by writing a model with quenched random disorder, based on orthogonal interaction matrices, which reproduces the high temperature expansion of the deterministic models. By using replica theory and well known results of integration on Lie groups we have been able to solve the model with quenched disorder. The model with quenched disorder has a replica symmetry breaking transition at a quite low temperature. The phase transition is discontinuous like in the random energy model.

We have also studied the low T phase. Even if the random model does not coincide with the deterministic model for all values of N down to $T = 0$ (since we know that for

Figure 12: As in fig. (11), but for the specific heat.

Figure 11: The internal energy as a function of T . Empty dots are from numerical simulations for the cosine model, $N = 806$. Crosses from numerical simulations for the model with quenched disorder, $N = 186$. The dashed line is for the static one step replica symmetry broken solution, the continuous line for the result obtained by imposing the marginality condition.

that the parameter for a low temperature expansion of the free energy is of the order of $\exp\{-\frac{6}{T}\}$. This means that the low temperature expansion is well convergent and has a free energy which differs from zero by a rather small amount in the whole region $T < T_C$. The high temperature free energy (given by (42)) and the low temperature free energy (which is equal to zero) intersect with an angle which is in agreement with the first order nature of the crystallization transition.

Dynamically our system is able to undergo a crystallization transition only for small values of N which satisfy the cardinality condition. If $(2N + 1)$ is prime and N is very large a local Monte Carlo annealing dynamics is unable to bring the system in its true ground state. The system remains in a metastable phase exactly like it does in the model with quenched disorder (where the zero energy ground state does not exist). In this regime the cardinality condition is irrelevant. This is illustrated by figures (11) and (12). We plot the energy and the specific heat versus T for the cosine model and for the model with quenched disorder (from numerical simulations), for the one step broken solution and for the marginality condition solution.

The model with quenched disorder has been conceived in order to reproduce the high T expansion of the deterministic model. Below the glass temperature T_G there are no *a priori* reasons why the two models should behave in a similar way. The fact that the two models coincide also in the metastable phase is clear from the results we show in figures (11), (12), and comes as a very nice surprise. One of the reasons for such a behavior is the fact that the metastable states in the two models have a very similar distribution, as we will show better in next section.

Also in case of the deterministic model, the metastable phase can be described using the marginality condition eq.(46) of the section 6.

Figure (11) shows that the solution where the marginality condition has been imposed describes very well the numerical results down to $T \sim 0.1$. Below that temperature the energy of the analytic solution departs from the numerical results reaching the static value ~ 0.063 at $T = 0$. This behavior is related to the fact that the breakpoint parameter m (as determined by imposing the marginality condition) is not proportional to T for low values of T . This fact will be discuss in better detail in the appendix and confirms the fact that the static replica equations are useful to predict the existence of the glassy transition at T_G but possibly not the full low T region.

The next section is devoted to describe the structure of the metastable states for the deterministic model at zero temperature by analyzing the numerical solution of the naive TAP equations. But for the existence of a crystalline state in case of prime $(2N + 1)$ prime the shape of the distribution of the metastable states will be shown to be similar to the one found in case of the random model.

Figure 10: Energy of the cosine model versus T , for prime values of $(2N + 1)$. The solid line is for decreasing T starting from a random configuration (and is the same for the two lattice sizes), while long dashes are starting from a true ground state for increasing T , $N = 44$, and dots for increasing T , $N = 806$.

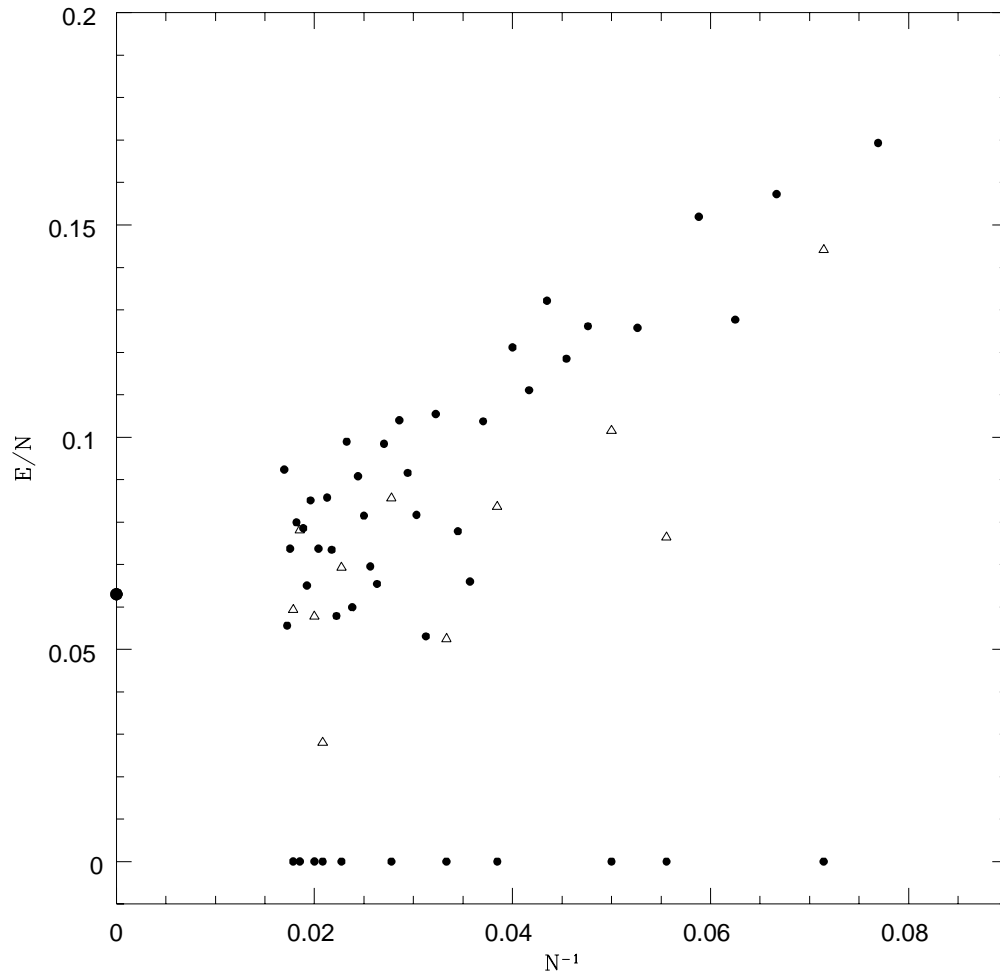


Figure 9: The ground state energy of the sine model divided by N versus N^{-1} for small values of N (at $N = \infty$ we plot the one step replica broken analytic result we have obtained for ground state of the model with quenched disorder). For $(2N + 1)$ prime we also plot the energy of first excited state with empty triangles.

8 Numerical Simulations of the Deterministic Model

We have studied the *cosine* model by using numerical simulations. We will start by presenting results which describe the nature of the ground state and illustrate the existence of a crystallization transition for values of N such that $(2N + 1)$ is prime. Then we will discuss the behavior of the internal energy and of the specific heat during an annealing process.

As we have discussed in section (2) the Hamiltonian (12) admits a zero energy ground state for values of N such that $(2N + 1)$ is prime. We have found the ground state by exact enumeration for small N values (see (A) for a detailed discussion of the technique). For higher values of N we have found the ground state by looking for solutions of the naive mean field equations, as we describe in the next section. For finding the ground state this method is slightly more efficient of the zero temperature Monte Carlo introduced in the previous section. In fig. (9) we plot the ground state energy divided by N versus N^{-1} for different values of N (at $N = \infty$ we plot the one step replica broken analytic result we have obtained for the ground state of the model with quenched disorder). For N such that $(2N + 1)$ is prime we also plot with a different symbol, the energy divided by N of the first excited state. The energy per spin is of order 0.1. The data of fig. (9) appear to be good evidence that for generic values of N the ground state energy tends to the value computed by the replica approach (we suggest to the curious reader to compare these results with the ones of (A), since the difference is easy to appreciate), and that the energy density does not vanish in the thermodynamic limit. The excited states for $(2N + 1)$ prime are a bit lower than the ground state for generic N values, but they do not seem to have an atypical behavior. In other words it would seem clear that the pathology of the prime values $(2N + 1)$ is confined to the ground state. The spectrum of the higher energy states, including the first excited state, does not depend on the cardinality of $(2N + 1)$.

For prime values of $(2N + 1)$ we find a crystallization first order transition for $T_C \sim 0.7$. Knowing the exact form of the ground state for such N values has been a remarkable plus. That allows us to study the system both starting from high T and cooling down to low T (in this case the system does never find the true ground states, but gets trapped at the energy of the metastable phase) and starting *from the ground state configuration*, slowly increasing the temperature T . We are able in this way to observe a thermal cycle we would not be able to detect in any other way. We show the results (for $N = 44$ and $N = 806$, both such that $(2N + 1)$ is prime) in fig. (10). The solid line is for decreasing T (and is the same for the two lattice sizes), while long dashes are for increasing T , $N = 44$, and dots for increasing T , $N = 806$.

We notice that the area included between ascending and descending curves increases with increasing N . The crystallization transition is of the first order, since the energy and the entropy are discontinuous at T_C . The discontinuities ΔE and ΔS are such that $\Delta E = T_C \Delta S$. The free energy vanishes approximately at T_C (see figure 1) and remains very close to zero below T_C in the crystalline phase. In fact at low temperatures the energy needed for a spin flip starting from the ordered ground state is in the range 6 – 10 so

Figure 8: Probability distribution of the energy of the metastable states for size $N = 30$ and 44 for the model with quenched disorder. The correct ground state energy is indicated with an arrow.

Figure 7: Energy of the model with quenched disorder versus T for $N = 100$. Different curves correspond annealing schedules.

Figure 6: As in figure (5), but for the specific heat. Here the continuous line is the static one step replica broken solution, while the dashed line is the prediction of (46) (inverting the notation of the former figure).

Figure 5: Energy of the model based on random orthogonal matrices versus T for $N = 186$. The dashed line is the static one step replica broken solution. The continuous line is the prediction of (46).

With limited computer time (on a reasonable workstation time allocation) we have been able to obtain reliable results for samples with a volume up to a few hundred spins.

In figure (5) we show our estimate for the internal energy on one disorder sample, for $N = 186$. In figure (6) we show the specific heat. We have started the run from high T and we have been decreasing the temperature at steps of .1.

We have tested that sample to sample fluctuations and finite-size corrections in the internal energy and heat capacity are negligible.

Our numerical results fit well the theoretical predictions for temperatures larger than $T_G \sim 0.5$. At T_G the system freezes. The energy does not decrease further than a value close to 0.12 and the specific heat decreases to a very small value. This is the dynamical transition we have discussed in the previous section. T_G is well above the temperature T_{RSB} and coincides with the transition point derived for the marginality condition.

The transition at T_G is of a dynamical nature. The system does not reach the lowest lying states (which have an energy close to 0.063). One could doubt if the freezing at $T_G \sim 0.5$ is a finite time effect. We show in fig. (7) the internal energy of the system as a function of T (here $N = 100$. We have used a value of N not too small in order to make the metastability visible). We plot three different curves for different run length. In the run with $t = 1000$, for example, we sweep the lattice 1000 times at each T point during our annealing procedure (i.e. while systematically decreasing T).

When the annealing time is too short for $T < T_G$ we get an energy that is too high. But as soon as the scheduling becomes slow enough we see that the energy thermalizes. The dynamical freezing appears to be a genuine behavior which survives in the limit of infinite times for large volumes. Let us note that for sizes less than $N \sim 50$ the system is able to find the ground state in a reasonable time on our simulation time scale, and we see it leaving the glassy phase. The limits $N \rightarrow \infty$ and $t \rightarrow \infty$ seem not to commute.

Finally we show in figure (8) the distribution probability for the energy of the metastable states at zero temperature for quite small system size (where we are able to reach the true ground state of the system).

For each lattice volume we have ran several millions of Monte Carlo runs at zero temperature (we sweep sequentially the lattice and we flip the local spin if so doing the internal energy decreases) starting from different initial conditions and searching for metastable states. We stop the search after we have found the lowest energy state 100 times. We take that as good evidence for having collected a fair sample of the low lying states. In fig. (8) we have also drawn an arrow locating the ground state energy given by eq.(44) (which is close to 0.063). The agreement with our zero temperature results is good. We also see that the distribution shape of the metastable states is reminiscent of that found in case of the SK model [20]. We will also see in the following that the energy distribution for the deterministic model is similar to the one of the model with quenched disorder (except for the existence of the very low lying ground state we have written explicitly for certain values of N).

Figure 4: Replica matrix sub-block size m as a function of T . The continuous curve is for the static value, the dashed curve is for the solution satisfying the marginality condition.

$$16\beta^2 G''(4\beta(1-q)) \langle \cosh(\sqrt{2\lambda}x)^{-4} \rangle = 1, \quad (46)$$

where the expected value is defined by

$$\langle A(x) \rangle = \frac{\int dx \frac{e^{-x^2}}{\sqrt{2\pi}} \cosh^m(\sqrt{2\lambda}x) A(x)}{\int dx \frac{e^{-x^2}}{\sqrt{2\pi}} \cosh^m(\sqrt{2\lambda}x)}. \quad (47)$$

We can find the dynamical transition point by maximizing the free energy under the marginality condition.

Maximizing the free energy (44) as a function of q for m fixed, under condition (45), we find that there are values of $m \leq 1$ such that eq. (46) is satisfied as soon as $T \leq T_{MC} \simeq 0.535 \pm 0.005$. This transition temperature is two times larger than T_{RSB} . We also get m and q as a function of the temperature. At T_{MC} q jumps discontinuously to a value $\simeq 0.962$. This value is smaller than the value we have found for the static solution. A priori we cannot expect the free energy derived using the marginality condition principle to a reasonable quantity, i.e. to satisfy the main inequalities of the thermodynamics. This is because we are in the wrong branch of the solutions of the replica equations, and we have not chosen m following a variational principle. For example the relation $u = \frac{\partial(\beta f)}{\partial\beta}$ is not satisfied for the marginality condition free energy. Also the value of the breakpoint parameter m (which we plot in fig. (4) together with the value from the static result) is not proportional to T at low temperatures.

It is not possible to describe the behavior of the system in the glassy phase without solving the full off-equilibrium equations, except for the value of the glassy temperature. As we have already discussed a complete analysis should not be confined to the case of one step replica symmetry breaking step. It would be very interesting to analyze the full low T behavior for a larger number of breaking steps, and eventually for a continuous breaking pattern. In the following sections we will present a numerical study of the model with quenched disorder and of the deterministic model. We will see that in both cases the system undergoes a dynamical transition at T_G , and that T_G is very close to the value T_{MC} we have computed here.

7 Numerical Simulations of the Disordered Model

The model with quenched disorder is based on symmetric orthogonal interaction matrices. In order to produce the interaction matrices needed in our simulations we started by generating a symmetric matrix with random elements with a Gaussian distribution. Starting from such a matrix we have obtained a symmetric orthogonal matrix by using the Graham-Schmidt orthogonalization procedure.

Such a model has an infinite range interaction, and Monte Carlo simulations are quite time consuming (but much less time consuming than for example p -spin models with $p > 2$).

for lower values of T a continuous symmetry breaking is needed to describe the system. This is what happens for the p -spin model [17]. As we will discuss in the next sections this second transition would probably have no relevance from the physical point of view, since the system is not able to explore the lowest free energy configurations. We will see that in an usual annealing process (i.e., a slow temperature cooling starting from a high temperature) the system has a transition at a temperature T_G well above the temperature T_{RSB} where replica symmetry breaks down. We will name the transition at T_G the *glass transition*. This transition is dynamical in nature and corresponds to the presence of a very large number of metastable states. At T_G the system remains trapped in a metastable state, and thermal fluctuations are very small.

6 The Marginality Condition

In the framework of mean-field theory it has been suggested that the solution to the Sompolinsky-Zippelius dynamical equations [18] undergoes a phase transition at a temperature T_G . Below that temperature the time-homogeneity hypothesis and the standard fluctuation-dissipation theorem are not valid. In the SK model the temperature T_G coincides with the transition point derived from the static approach, where the replica symmetric solution becomes unstable. It has also been suggested that this temperature coincides with the temperature T_{MC} where a one step replica broken solution to the mean field equations exist such that the size of the replica matrix sub-block m is fixed by the condition that the replicon eigenvalue vanishes. This has been called the *marginality condition* [19].

More recently several authors have investigated the p -spin spherical spin glass model [14]. In this case it is possible to write closed expressions for the correlation and response functions in the off-equilibrium regime. It has been noted [15] that the dynamical equations undergo a glass transition at a temperature T_G where the relaxational dynamics slows down and aging effects start to appear. The temperature T_G is larger than the transition point where replica symmetry breaks down, as predicted by the static approach. This is a consequence of the stability of the replica symmetric solution and corresponds to the fact that at the transition point the spin-glass order parameter $q(x)$ is discontinuous. In this model T_G coincides with T_{MC} .

The models we are describing in this work (the model with quenched random disorder as well as the deterministic one) are good candidates for a test of the marginality condition principle. The main reason is that at the transition point the order parameter q jumps discontinuously to a value extremely close to 1. The system essentially freezes and the difference between the static transition temperature T_{RSB} and the dynamical transition temperature value T_G is large. In the following sections we will use numerical simulations to show that, for reasons not completely clear to us, the principle seems to work well.

Now we want to derive the value of T_{MC} in our particular case. We start from eq.(38) and we compute the Hessian matrix in the Λ, Q space. The interested reader can find the technical details in the appendix. The marginality condition gives

Figure 3: As in fig. (1), but for the entropy of the system. Here again the dotted line is solely meant to indicate the zero. The entropy of the one step solution is very small in the low T phase.

Figure 2: As in fig. (1), but for the internal energy of the system.

Figure 1: Free energy of the model with quenched random disorder versus T . The continuous line is the replica symmetric solution, the dashed line is the one step replica broken solution. With the dotted line we only indicate the zero of the free energy. The free energy vanishes at $T \sim 0.71$.

We plot the replica symmetric free energy found in eq. (42) in fig. (1) (together with the one step replica broken result we will compute in the following).

In fig. (2) we plot the internal energy and in fig. (3) the entropy of the system.

In the high-temperature region the quenched and the annealed solutions coincide as usual for long range models.

The replica symmetric solution is stable at all temperatures. But since for $T \leq 0.26$ it gives a negative entropy (see fig. (3)) it cannot be correct down to $T = 0$. We expect replica symmetry to break above (but very close) to $T = 0.26$. Here the system enters a glassy phase very similar to that of the random energy model [13] and of the p -spin systems (see for example [14, 15]).

We can compute the one step replica broken solution. We parameterize the matrices Q and Λ in the usual way. In presence of an uniform magnetic field the matrix elements Q_{ab} take the value q if a and b belong to the same sub-block of size m , while they take the value q_0 if they do belong to different sub-blocks. We parameterize the matrix Λ_{ab} with blocks of the same size m , and we set its elements equal to λ or λ_0 with the same procedure we used for Q . We consider here the simpler case of zero magnetic field, where the parameters q_0 and λ_0 are zero and we set

$$Q_{a,b} = q \quad (a \neq b), \quad \Lambda_{a,b} = \lambda \quad (a \neq b) \quad (43)$$

inside the blocks of size m ($Q_{aa} = 1; \Lambda_{aa} = 0$). After some algebra we obtain

$$\begin{aligned} \beta f = & 2\beta - \frac{1}{2m} [(m-1)G(4\beta(1-q)) + G(4\beta(mq+1-q))] \\ & + \lambda q(m-1) - \log(2) + \lambda - \frac{1}{m} \log \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} ch^m(\sqrt{2\lambda}x). \end{aligned} \quad (44)$$

The stationary equation for q tells us that

$$\lambda = \frac{2\beta}{m} [G'(4\beta(mq+1-q)) - G'(4\beta(1-q))]. \quad (45)$$

We can use this relation to eliminate λ from (44). We are left with a function of q and m , and we have to find a stationary point. This expression cannot be solved in close form. We have plotted the numerical solution with dashed lines in figures (1), (2), (3).

At $T_{RSB} \sim 0.26$ there is a phase transition to a phase with broken replica symmetry. At the transition point T_{RSB} the value of the entropy is finite but very small (~ 0.0004), the value of q jumps discontinuously to a value very close to 1 (~ 0.9998), and λ is large but finite (~ 10) (in the Random Energy Model at the transition point $q = 1$ and $\lambda = \infty$ [16]). Below T_{RSB} the parameter m is very approximately proportional to T , $m = 1$ at T_{RSB} . This is the typical scenario for a large class of models where the order parameter jumps discontinuously at the transition.

We have not studied in detail the stability properties of the replica broken solution. It is possible that the one step solution is stable down to a very low temperature, and that

$$\prod_{a,b=1}^n \delta\left(\sum_{j=1,N} \sigma_j^a \sigma_j^b - N Q_{a,b}\right) \simeq \int \prod_{a,b=1}^n d\Lambda_{a,b} \exp\left\{i \sum_{a,b} \Lambda_{a,b} \left(\sum_{j=1,N} \sigma_j^a \sigma_j^b - N Q_{a,b}\right)\right\}. \quad (36)$$

After a little more algebra (very similar to the one developed in (A)) we find that

$$\overline{Z}^n = \int dQ d\Lambda \exp(-N A[Q, \Lambda]). \quad (37)$$

In the large N limit the free energy is obtained by finding the saddle point value of $A[Q, \Lambda]$, which has the form

$$A[Q, \Lambda] = -\frac{1}{2} \text{Tr} G(2\beta Q) + \text{Tr}(\Lambda Q) - F(\Lambda), \quad (38)$$

where G has been already defined, and

$$F(\Lambda) \equiv \ln \sum_{\sigma^a} \exp\left\{\sum_{a,b} \Lambda_{a,b} \sigma^a \sigma^b\right\}. \quad (39)$$

We will need to study eq. (38) to discuss the solutions of the model.

5 Saddle Point Equations and Replica Symmetry Breaking

In the previous section we have found the saddle point equations which allow to solve the model with quenched disorder defined in (13). Let us recall that the free energy (multiplied times $n\beta$) in terms of the matrices Q and Λ is

$$\beta f_O = \lim_{n \rightarrow 0} \frac{A[Q_{SP}, \Lambda_{SP}]}{n}, \quad (40)$$

where A is defined in (38), and Q_{SP} and Λ_{SP} are evaluated at the saddle point of A .

The free energy (14) of the model with quenched random disorder (which has the same high-temperature expansion than the deterministic one (1,3)) is given by

$$\beta f = 2\beta - 2\beta f_O(2\beta). \quad (41)$$

Let us start by considering the annealed case, $n = 1$. Here the matrix Σ is set equal to 1. The action does not depend on Λ , and we find for the free energy density and the internal energy

$$\begin{aligned} f &= 2 - \frac{1}{2\beta} G(4\beta) - \frac{1}{\beta} \log(2), \\ e &= 2(1 - G'(4\beta)) = 2 - \frac{\sqrt{1 + 64\beta^2} - 1}{4\beta}. \end{aligned} \quad (42)$$

D_σ can be interpreted as the distance of the configuration σ from the subspace F . The relation $P_\sigma^2 + D_\sigma^2 = 1$ holds. The Hamiltonian (14) can be written now as $4D_\sigma^2$. The ground state energy is given by the minimum distance D_m of one of the 2^N configuration from the random subspace. This problem is well studied in the case $\nu N = 1$, i.e. in the limit $\nu \rightarrow 0$, mainly for its applications to perceptrons [11], but it has not been discussed in the most general case.

For $\nu = 1/2$ by inverting the second relation after some algebra we find (we omit the suffix $\nu = \frac{1}{2}$ for G and ψ)

$$G(z) = \int_0^1 dt \frac{\sqrt{1 + 4z^2 t^2} - 1}{2z}, \quad (30)$$

which gives

$$G'(z) = \frac{\psi(z) - 1}{z}. \quad (31)$$

After integrating the last relation with the condition $G(0) = 0$ we find

$$G(z) = \frac{1}{2} \log(\sqrt{1 + 4z^2} - 1) - \frac{1}{2} \log(2z^2) + \frac{1}{2} \sqrt{1 + 4z^2} - \frac{1}{2}, \quad (32)$$

where the constant term has been chosen such that $G(0) = 0$.

We have already said that we have obtained this G for V unitary. It is easy to argue that when we integrate over orthogonal matrices the only difference is that $G(\beta z)$ gets substituted from $\frac{1}{2}G(2\beta z)$. That can be seen for example by noticing that the function G has to be the same in the two cases (since the same diagrams contribute) and at first order in β orthogonal and unitary matrices have to give the same results. So the only allowed renormalization will be of the kind $G(z) \rightarrow \alpha G(\frac{z}{\alpha})$. The counting of the eigenvalues leads to the conclusion $\alpha = \frac{1}{2}$.

Using the fact that for integer positive k

$$\text{Tr} \left(\frac{\beta \Omega}{N} \right)^k = \text{Tr} (\beta \Sigma)^k, \quad (33)$$

where the matrix Σ is defined as

$$\Sigma_{a,b} \equiv \sum_{k=1}^N \sigma_k^a \sigma_k^b, \quad (34)$$

it follows immediately that

$$\text{Tr} G \left(\frac{\beta \Omega}{N} \right) = \text{Tr} G(\beta \Sigma). \quad (35)$$

To continue our computation we insert a δ -function, and introduce the Lagrange multipliers Λ with the representation

The value of G is given in [12] (when, as we already said, the integral is over the unitary matrices). Following [12] let us define the generating function for the traces of D as

$$\Phi_D(j) \equiv \frac{1}{N} \sum_{k=0}^{\infty} j^k \text{Tr} D^k , \quad (22)$$

in the case where $d \equiv \text{Tr} D = 0$. If $d \neq 0$ we define the generating functional as

$$\Phi_D(j) \equiv \frac{1}{N} \sum_{k=0}^{\infty} j^k \text{Tr} (D - d)^k , \quad (23)$$

that allows a straightforward generalization of the computation, by only adding an additional contribution to the free energy. We define the function z_D as

$$z_D(j) \equiv j \Phi_D(j) , \quad (24)$$

and finally we define the function $\psi_D(z)$ by

$$\psi_D(z) \equiv \Phi(j_D(z)) , \quad (25)$$

where $j_D(z)$ is obtained by inverting (24). All said, [12] tells us that G is given by

$$G_D(z) = \int_0^1 dt \frac{\psi_D(zt) - 1}{t} . \quad (26)$$

In the orthogonal symmetric case $O^2 = 1$ and the eigenvalues of D can take the values ± 1 . As far as our problem is concerned we are interested in the case where half of the eigenvalues take the value $+1$ and half the value -1 . We will discuss here a more general case, where a fraction ν of the eigenvalues is $+1$ and a fraction $1 - \nu$ is -1 .

It is interesting to notice that the ground state of the model has a simple geometrical significance. Let us consider our series of N spins σ , and look at it as one of the vertices of the unit hypercube in N dimensions. Let us imagine such an hypercube as embedded in \mathfrak{R}^N . Now we extract a random linear subspace F of dimension νN , which includes the origin. For example if we have $N = 2$ spins the configuration will seat on one of the four corners of a 2 dimensional square, and for $\nu = \frac{1}{2}$ we would pick a random line passing through the origin. If P is the projector of F the matrix O is given by

$$O = 2P - 1 . \quad (27)$$

We define the norm of the projection of a spin configuration $\{\sigma\}$ over the subspace F by

$$P_\sigma = |P\sigma| , \quad (28)$$

and the norm of the projection over the complementary subspace F^-

$$D_\sigma = |(1 - P)\sigma| . \quad (29)$$

4 The Replica Approach

By using replica theory techniques [7, 8] we will solve now the model with quenched disorder defined by the Hamiltonian (13). As usual we define the free energy of n replicas as

$$f^{(n)}(\beta) \equiv \lim_{N \rightarrow \infty} \left(-\frac{1}{\beta N} \overline{Z_O(\beta)^n} - 1 \right), \quad (15)$$

where with the bar we denote the average over the quenched disorder and

$$Z_O^n \equiv \sum_{\{\sigma^a\}} \exp \left\{ -\beta \sum_{a=1}^n H_O^a \right\}. \quad (16)$$

We have to average over the quenched disorder. To this end we have to compute

$$\overline{Z_O^n} = \int dO \exp \left\{ \sum_{k,j=1}^N \beta \Omega_{k,j} O_{k,j} \right\}, \quad (17)$$

where the integral runs over orthogonal symmetric matrices, and

$$\Omega_{k,j} \equiv \sum_{a=1}^n \sigma_k^a \sigma_j^a. \quad (18)$$

We will show now that we can solve a more general problem considering a symmetric coupling matrix with some quite general preassigned eigenvalue distribution. We will derive such more general form. We will eventually obtain the relevant result specializing this general form to orthogonal symmetric matrices.

A generic real symmetric matrix O can be decomposed as²

$$O = V D V^*, \quad (19)$$

where D is a diagonal matrix which controls the spectrum of O , and V is the orthogonal matrix which diagonalizes O . By using this decomposition we have to compute

$$\overline{Z_O^n} = \int dV \exp \{ \text{Tr}(\beta V \Omega_{k,j} V^* D) \}, \quad (20)$$

where D is a diagonal matrix, dV is the Haar invariant measure over the orthogonal group, and the matrix Ω is defined in (18). We can use the results derived in [12] for unitary matrices and adapt them to the orthogonal case. So, let us assume for a while that we are integrating over unitary matrices V . Using the fact that Ω has finite rank we find that

$$\int dV \exp \{ \text{Tr}(\beta V \Omega_{k,j} V^* D) \} = \exp \{ N \text{Tr} G_D \left(\frac{\beta \Omega}{N} \right) \}. \quad (21)$$

²We like to stress with * the operation of hermitian conjugation, which for real matrices coincide with transposition.

3 The Disordered Model

It is natural to introduce at this point a model which contains quenched disorder. The companion paper (\mathcal{A}) justifies in detail this approach. By studying a suitable disordered model we try to understand how general is a very specific 2-spin interaction like for example the sine one (1). We will find they have indeed much in common, and that the random model allows to reconstruct exactly the most part of the phase diagram. As before we define the Hamiltonian (here O stands for orthogonal)

$$H_O \equiv \sum_{x,y=1}^N O_{x,y} \sigma_x \sigma_y , \quad (13)$$

where now $O_{x,y}$ is a generic orthogonal symmetric matrix. The same behavior of the deterministic model will be obtained by using a rescaled Hamiltonian

$$\tilde{H}_O \equiv 2N - 2H_O . \quad (14)$$

The form we have just written is important since also in the case of the original sine and cosine models the Hamiltonians defined after eq.(12) can be written in the form $2N - 2\sum_{i,k} M_{i,k} \sigma_i \sigma_k$, by neglecting terms which are irrelevant in the $N \rightarrow \infty$ thermodynamic limit.

The first element for the comparison of the two class of models, the sine and cosine versus the random one, can be obtained from noticing general features of the high temperature expansions of the models. For both class of models the couplings¹ are of order $N^{-\frac{1}{2}}$. The diagrams which contribute to the infinite volume limit have the same topology for the two classes of models, and they only depend on quantities like the trace of the couplings to positive powers, which have been built to be equal in the two classes of models.

The reasoning of the former paragraph proves that sine and cosine models defined from (1) and (3) and the model with quenched disorder defined from (14) have the same high temperature expansion. On the other side we have exhibited a ground state of the deterministic system which exists for prime values of $(2N + 1)$. Such construction obviously does not apply to the disordered models. This implies that the static properties of the two class of models (for prime values of $(2N + 1)$) cannot coincide all the way down to $T = 0$. There is a crystallization transition only in the deterministic models, thanks to very peculiar cardinality properties of N .

We will give evidence that the random and the deterministic model do coincide at all temperatures in the metastable phase. This is the case for generic values of N , since as we already stressed the cardinality of $2N + 1$ is irrelevant for the behavior of the deterministic model in the metastable phase. A similar pattern could hold for the low autocorrelation model, but in the present case of the 2-spin interaction the analysis is far simpler, and we are able to carry it through all the way.

¹This is not true for all soluble spin glass models. In the dilute models the average coordination number z remains finite and the couplings may be quantity of order 1, with a probability of order $\frac{z}{N}$.

in (\mathcal{A}) to show that replica theory can be a reasonable tool to investigate deterministic models.

It is remarkable that for prime values of p , such that $p = 4n + 3$, it is possible to exhibit in an explicit way one ground state of the system. Let us construct such ground state configuration. Following Legendre [10] we set $\sigma_p = 0$ and

$$\sigma_j = j^{\frac{1}{2}(p-1)} \bmod p . \quad (10)$$

In this way σ_j is $+1$ or -1 , if $j < p$. Indeed a theorem by Fermat [10] tells us that if j is not multiple of p , $j^{(p-1)} = 1, \bmod (p)$ and therefore $j^{\frac{1}{2}(p-1)} = \pm 1$.

We will evaluate the energy of this sequence and only at the end we will impose that $\sigma_p = \pm 1$ on the last site p . It is well known that for this sequence all the correlations C_k are equal to -1 [10]. It is also remarkable (and the crux of this paper) that on such a sequence the Fourier transform is given by

$$B(k) = G(p) \sigma_k , \quad (11)$$

where, according to Gauss [10], $G(p) = 1$ for $p = 4n + 1$ and $G(p) = -i$, for $p = 4n + 3$. This Gauss theorem makes easy to verify that the configurations we have exhibited have energy 1 (the lowest possible energy for odd values of p). Now we change the last spin to ± 1 . It is easy to verify that after doing that the energy of configurations with p of the form $4n + 3$ stays unchanged to 1, while for $p = 4n + 1$ the energy grows to 5. It is clear now that for p prime of the form $4n + 3$ we have exhibited a true ground state of the low autocorrelation model.

By using Gauss theorem about Fourier transforms of Legendre sequences we are able now to define a simple model with 2-spin interaction which has the same ground state of the 4-spin interaction low autocorrelation model. We are ignoring here the presence of the spin with value zero. The new Hamiltonian has the form

$$H = \sum_x |G(p) \sigma_x - B(x)|^2 . \quad (12)$$

We can further simplify the model by noticing that the sequence of the σ in the ground state we have written is symmetric or antisymmetric around the point $\frac{p-1}{2}$, depending on the value of $G(p)$. That allows us to define two new models with half the number of degrees of freedom which continue to admit (for selected p values) the ground state we have written. Such two models are exactly the sine and the cosine model we have define in our introduction.

Hopefully we have given clarifying hints about the nature of our two models. Now we can proceed to study them.

discuss the mean field equations for the deterministic models. In section (10) we draw our conclusions. In the final appendix we present the technical details of a computation concerning the marginal stability.

2 The Genesis of Our Models

In order to introduce the models we have defined in the previous section, and which we will study in the following, let us recall some basic definitions from (\mathcal{A}), and repeat briefly the reasoning which leads to exhibit the exact ground state of the model for some particular values of the number of spins. The reader in need of further details should consult (\mathcal{A}) and [10].

The low autocorrelation model is based on sequences of length p of spin variables $\sigma_x = \pm 1$, with $x = 1, p$, and on the Hamiltonian

$$H = \frac{1}{p-1} \sum_{k=1}^{p-1} C_k^2, \quad (5)$$

where the C_k are the correlations at distance k , defined as

$$C_k \equiv \sum_{j=1}^p \sigma_j \sigma_{j+k}, \quad (6)$$

where we are taking periodic boundary conditions (this is, in the terminology of (\mathcal{A}), the *periodic* model), i.e. the indices are always summed modulo p . In this way the indices which address the σ variables always belong, as they should, to the interval $[1, p]$. It is useful to rewrite the Hamiltonian as

$$H = \frac{1}{p-1} \sum_{k=1}^p (|B(k)|^4 - 1) + 1, \quad (7)$$

where the Fourier transform is defined as

$$B(k) \equiv \frac{1}{\sqrt{p}} \sum_{x=1}^p e^{i \frac{2\pi k}{p} x} \sigma_x, \quad (8)$$

and i is the imaginary unit. The thermodynamics of the model can be reconstructed thanks to the partition function at inverse temperature $\beta \equiv \frac{1}{T}$ in the volume p

$$Z_p(\beta) \equiv \sum_{\{\sigma\}} e^{-\beta H\{\sigma\}}. \quad (9)$$

An interesting way to look at the Hamiltonian (5) is to consider it as a particular form of a fully frustrated 4-spin interaction. Here only the 4 spin terms which are contained in a square of two points correlation functions appear. This point of view has been useful

$$C_x(\sigma_y) \equiv \frac{1}{\sqrt{N}} \cos\left(\frac{2\pi xy}{N}\right) \sigma_y. \quad (4)$$

Let us anticipate a discussion of the phase diagram of the model. We will see that a very important role is played by the case where $(2N + 1)$ is prime (and N is odd for the sine model and it is even for the cosine model). In this case the thermodynamical limit of the partition function is anomalous. We will show indeed that from the thermodynamical point of view for prime values of $(2N + 1)$ our models undergo a first order transition at temperature T_C . We find such *crystallization* transition only in the case of prime $(2N + 1)$. At T_C the system goes from a disordered state to an highly ordered one. The specific heat in the low temperature crystalline state is extremely small.

The system however has a metastable phase whose internal energy is regular at T_C . When we start from high T with a local Monte Carlo dynamics, and we decrease T with some kind of annealing procedure, we pass through T_C without any noticeable change in the thermodynamical quantities.

At a lower temperature T_G , within the metastable phase, there is a transition to a *glassy* phase (a second order phase transition). This transition exists for generic values of N . In the glassy phase the system may exist in many different equilibrium metastable states. Here there are many states which survive with finite probability in the infinite volume limit (in other words replica symmetry is broken). In this phase the system freezes and thermodynamic fluctuations (for instance of the energy and of the magnetization) are very small. The behavior of the system at the glass transition can be understood in the framework of replica theory. It is remarkable that the glass transition temperature T_G is the temperature where the entropy in the metastable phase becomes nearly equal to the entropy in the glassy phase (i.e. very close to zero).

We stress again that the crystalline phase exists only for $(2N + 1)$ prime, N odd for the sine model and even for the cosine model. On the other hand the behavior of the system in the high temperature phase and in the metastable phase is generic, and does not depend on the cardinality of $(2N + 1)$.

In section (2) we will briefly describe the genesis of this model, after our paper (\mathcal{A}). We will also discuss the low T phase of the low autocorrelation model, mainly by using number theory. We will again be quite sketchy, inviting the interested reader to consult (\mathcal{A}) for a more detailed discussion. In section (3) we will define a model containing quenched disorder, which we will eventually dissect by replica theory, and show to give a fair description of many features of our deterministic models. We will eventually show that basically the random model and the deterministic one do coincide, a part for minor details like the non-generic existence of the crystalline phase in the deterministic models.

In section (4) we describe our replica computation. In section (5) we analyze the saddle point equations. We describe the replica symmetric and the one step replica broken solution. In section (6) we discuss the so-called marginality condition. In section (7) we illustrate our numerical simulations of the models with quenched random disorder, and in section (8) the numerical simulations of the deterministic models. In section (9) we

1 Introduction

In a recent companion paper [1] (which in the following we will quote as (\mathcal{A})) we have started (at the same time than Jean Philippe Bouchaud and Marc Mezard in [2]) a study of the role of replica field theory when applied to the study of systems which *do not* contain quenched disorder (for further connected work which helps clarifying this issue see [3, 4]).

The immediate starting point which prompted our investigation (\mathcal{A}) was a model of binary sequences with low autocorrelation, as originally discussed from Golay and Bernasconi [5, 6]. The model was for us a prototype of a system which does not contain quenched random disorder, but has an interesting spin-glass like low T structure (for general discussions about disordered systems, see [7, 8, 9]). We have shown that replica theory allows to gather information about the full phase diagram of the theory, excluding only the very low T behavior, which is determined by various factors, including the cardinality of the number of spins of the system, N . We have indeed shown in (\mathcal{A}) that replica theory can allow a study of the full deterministic model, and does not have to be limited to an approximated form.

Apart from such a direct application, we have discussed in (\mathcal{A}) a more general valence of such an approach. The ability of investigating deterministic systems with a complex landscape is an important bonus. We also stress that we are still lacking a comprehensive description of the glass state, and that such an approach seems a good candidate to this task.

In the following we will discuss a new class of models without quenched disorder. They derive quite directly from the ones studied in (\mathcal{A}), by noticing the peculiar role the Fourier transform is playing (we will discuss this point in some detail in section 2). We will find that these models behave in a way that appears to be relevant to the description of the glass state.

We will define the first model (the *sine model*) by the Hamiltonian

$$H_S \equiv \sum_{x=1}^N \left\{ \sum_{y=1}^N [S_x(\sigma_y)] - \sigma_x \right\}^2, \quad (1)$$

where

$$S_x(\sigma_y) \equiv \frac{1}{\sqrt{N}} \sin\left(\frac{2\pi xy}{N}\right) \sigma_y, \quad (2)$$

and the spin variables σ_x take the values ± 1 . We define the analogous *cosine model* by the Hamiltonian H_C

$$H_C \equiv \sum_{x=1}^N \left\{ \sum_{y=1}^N [C_x(\sigma_y)] - \sigma_x \right\}^2, \quad (3)$$

where

Replica Field Theory for Deterministic Models (II): A Non-Random Spin Glass with Glassy Behavior

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Abstract

We introduce and study a model which admits a complex landscape without containing quenched disorder. Continuing our previous investigation we introduce a disordered model which allows us to reconstruct all the main features of the original phase diagram, including a low T spin glass phase and a complex dynamical behavior.

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