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Memorizing polymers' shapes and permutations

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Abstract. We discuss the equilibrium configurations of heteropolymers. The interaction potential for each pair of monomers is chosen in such a way (using a 'Hebbian' learning rule) that the (meta)stable states of the polymer are some preassigned shapes. The problem is analysed in some detail in the infinite-dimensional case, where the 'shapes' correspond to permutations, and the memory capacity is computed. The one-dimensional case is also considered.

1. Introduction

The protein-folding problem deals with the prediction of the native shape of a protein, starting from the 'first principles', i.e. the form of the interactions of the monomers between themselves and with the solvent. While most proteins seem to have only one or a few equilibrium shapes, it is possible that one could 'build' a heteropolymer which might have many possible equilibrium (or metastable) shapes, completely different from one another. This may happen if one chooses the interactions between pairs of monomers in the chain in an appropriate way. We shall show that, at least for polymers living in an infinite-dimensional space, it is possible to memorize many distinct globular shapes in a single chain, provided one can choose arbitrarily the interaction potentials between pairs of monomers. A Hebbian learning rule inspired from the one used in memory neural networks [1] can then provide the appropriate pair interactions for a proper memorization. The actual shape adopted by the polymer at low temperatures will depend on the initial conditions: in the best situation the polymer will relax to the nearest (in some sense) shape which has been memorized in the pair potential. This idea of memorization is basically identical to the one which has been introduced by Hopfield [2] for neural networks. The basic difference is in the nature of the device: here the analogue of a configuration of neurons is a configuration of the polymer. The memorized patterns are some special polymer configurations (shapes), and the memory is contained in the pair-interaction potentials.

More specifically, let us consider a polymer chain of N monomers in a D-dimensional space. In a given configuration of the chain, the position of monomer

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number τ ($\tau \in 1, \ldots, N$) is called x_τ. We neglect the interactions with the solvent and describe the chain by the Hamiltonian

$$H = \sum_{\tau=1}^{N} g(x_\tau - x_{\tau+1}) + \sum_{\sigma,\tau=1}^{N} V_{\tau\sigma}(|x_\tau - x_\sigma|) \tag{1}$$

where g represents the 'linear memory', which could be taken for instance as $g(x) = x^2$, and $V_{\tau\sigma}$ is what we call the pair potential, the interaction between each pair of monomers σ, τ which are not neighbours along the chain. Given p shapes x_τ^μ ($\mu \in 1, \ldots, p$) which one wants to memorize, it may be possible, if p is not too large, to find a set of pair potentials $V_{\tau\sigma}(r)$ such that all the shapes will be (meta-) stable configurations of the Hamiltonian H. This very interesting problem has been introduced and discussed by Sasai and Wolynes [3], who call the resulting Hamiltonian an associative memory Hamiltonian for protein folding. Here we formulate it in somewhat more general terms, especially because we do not restrict the space of interactions as interactions between a small number of monomer types (for instance hydrophobic and hydrophillic), so that we have potentially more possibilities for the application of these systems in pattern recognition. Although we have been able to perform the computation only in two extreme cases where D is equal to one or infinity, we would like to briefly present a simple lattice version of the general Sasai-Wolynes problem and write down some hypothetical form of the pair potential. We are interested in globular polymers. One could use a short-range pair potential with excluded volume effect together with a short-range attraction. After discretizing the problem on a lattice, it looks reasonable to try to memorize one shape x_τ^μ by strengthening the attraction between monomers τ and σ (lowering $V_{\sigma\tau}(1)$) whenever monomers σ and τ are lattice neighbours in the shape x_μ. If interference effects are not too severe, the memorization of several shapes might then be obtained by a kind of Hebbian rule like

$$V_{\sigma\tau}(0) = V_0 \qquad V_{\sigma\tau}(1) = -V_1 - V_1' \sum_\mu \delta(|x_\tau^\mu - x_\sigma^\mu|, 1) \qquad V_{\sigma\tau}(r) = 0 \quad r > 1 \tag{2}$$

where V_0, V_1, V_1' are positive constants. It would be quite interesting to see (perhaps through some numerical simulations) if such a system (or one with longer-range interactions) could memorize some shapes in two or three dimensions. In this paper we shall not say anything about this general problem. We shall study analytically two extreme versions of this problem.

(1) The infinite-dimensional case: each monomer is then the neighbour of every other monomer. A configuration is a permutation of all the sites, and the learning rule 2 has to be adapted to this case. This problem, which will be analysed in the next section, presents many similarities to the memorization in neural networks [1], except that the basic configurations are permutations.

(2) The one-dimensional case: if the self-avoidance is not strict, the problem of memorizing one shape in one dimension is not trivial. In section 3 we shall study a 'directed' version of this problem.

Before proceeding we would like to mention previous works which are related to the present one in some aspects. De Gennes [4] has studied the memorization of one shape by imprinting it in some external substrate. The memory is then encoded in an external potential which acts on the polymer, while here we study the case where the memory is encoded in the pair potentials. The problem of random heteropolymers on the fully connected lattice has been considered by Garel and Orland [8], but they have not addressed the question of shape memorization.

2. 'Shapes' on the fully connected lattice and permutations

It is a common procedure in statistical mechanics, in order to gain some insight into difficult problems, to define toy models solvable by mean-field technique. A general situation is that problems that are very difficult when formulated in finite-dimensional spaces simplify in the 'infinite-dimensional space limit', to be understood as a space where all points are the same distance from each other.

Here we want to study the memorization of folded sequences in such a space. We consider N points, labelled by i, $i=1,\ldots,N$ and chains of N 'monomers' labelled by τ, $\tau=1,\ldots,N$ that completely fill the space. A given sequence in space, specified by the position of all monomers $\tau=\tau(i)$, can be identified with a permutation π of indices i. For each permutation π we define a permutation matrix $S_{i\tau}^{\pi}$

$$S_{i\tau}^{\pi}=\begin{cases}1 & \pi(\tau)=i\\ 0 & \text{otherwise}\end{cases} \tag{3}$$

that verifies

$$\sum_{i} S_{i,\tau}^{\pi}=\sum_{\tau} S_{i,\tau}^{\pi}=1. \tag{4}$$

Given two permutations π, π' we can define the overlap as the number of sites where $\pi(\tau)=\pi'(\tau)$

$$q^{\pi,\pi'}=\frac{1}{N}\sum_{i,\tau} S_{i,\tau}^{\pi}S_{i,\tau}^{\pi'}. \tag{5}$$

Our aim is to store, by means of a Hamiltonian function of the variables $S_{i\tau}$, a given set of p permutations, represented by the matrices $\xi_{i\tau}^{\mu}$, $\mu=1,\ldots,p$ chosen at random, independently, and with uniform probability out of the $N!$ possibilities. It looks natural in this context to use a Hamiltonian of the kind

$$H=-\frac{1}{2}\sum_{i\tau,j\sigma} J_{ij}^{\tau\sigma}S_{i\tau}S_{j\sigma} \tag{6}$$

and to take as coupling matrix $J_{ij}^{\tau\sigma}$ a Hebbian form similar to the one introduced by Hopfield [2] for memory networks:†

$$J_{ij}^{\tau\sigma}=A\sum_{\mu=1}^{p}\xi_{i\tau}^{\mu}\xi_{j\sigma}^{\mu}. \tag{7}$$

This gives

$$H=-\frac{A}{2}\sum_{\mu=1}^{p}\left(\sum_{i\tau} S_{i\tau}\xi_{i\tau}^{\mu}\right)^2. \tag{8}$$

A few comments are in order:

In Ising systems, where the dynamical variables take the values $S_i=\pm 1$, the terms of the kind $J_{ii}S_i^2$ are irrelevant in the Hamiltonian. Here they are present and contribute to H with a term $-\frac{1}{2}A\,\Sigma_{\mu}\,\Sigma_{i\tau}\,S_{i\tau}\xi_{i\tau}^{\mu}$.

† It is interesting to note that a Hamiltonian similar to (6) has been considered in [5] to study the travelling salesman problem. The same problem is formulated in terms of Potts variables in [6] and [7].

The constant A in H has to scale with N in such a way that the entropy and the energy will be of the same order [10]. As the number of states is $N!$, the entropy is $\sim N \ln N$ and the correct choice for A is (choosing a scale for the energy) $A = \ln N / N$; accordingly the free energy 'density' will be written as

$$F = -\frac{T}{N \ln N} \ln Z. \tag{9}$$

It could be possible to take into account the linear structure of the chain introducing an interaction between monomers occupying adjacent places along the chain, of the kind $B \Sigma_{ij\tau} K_{ij}^{\tau} S_{i\tau} S_{j\tau+1}$. If B is taken of the same order of magnitude as A, such a term is irrelevant in the thermodynamical limit. We leave for future investigation the study of the role of this kind of term when B is scaled in such a way as to give rise to a relevant term.

The coupling matrix we introduced in (6) and (7) depends on the positions (i, j) of the monomers in the space. This cannot be avoided in a non-trivial model in an infinite-dimensional space, where constraint (4) holds.

In the next subsection we will study the memorization of a single sequence $\xi_{i\tau}$. In that case we can always choose $\xi_{i\tau} = \delta_{i\tau}$ by a gauge (Mattis) transform of the kind

$$J_{ij}^{\tau\sigma} \to J_{ij}^{\pi(\tau)\pi(\sigma)} \qquad S_{i\tau} \to S_{i\pi(\tau)} \tag{10}$$

We obtain in this way

$$H = -\frac{\ln N}{2N} \left(\sum_i S_{ii} \right)^2. \tag{11}$$

In section 2.3 we will study the more complicated case of $p \gg 1$ patterns, where the replica trick is needed to average over the random patterns.

2.1. The one-pattern case

In the one-pattern case the partition function can be written in a closed form for any value of N. The partition function can be written as

$$Z = \sum_{\{S_{i,\tau}\}} \exp\left[\beta \frac{\ln N}{2N} \left(\sum_i S_{i,i} \right)^2 \right] = \int \frac{dm}{\sqrt{2m/\beta N \ln N}} e^{-\beta N \ln N m^2/2} \sum_{\{S_{i,\tau}\}} e^{\beta m \ln N \Sigma_i S_{ii}} \tag{12}$$

We expand in high-temperature series, compute the sum over the Ss, and re-sum the expansion:

$$\sum_{\{S_{i,\tau}\}} e^{\beta m \ln N \Sigma_i S_{ii}} = \sum_{k=0}^{N} \zeta^k \sum_{i_1 < i_2 < \ldots < i_k} \sum_{\{S_{i,\tau}\}} S_{i_1,i_1} \ldots S_{i_k,i_k}$$

$$= \sum_{k=0}^{N} \zeta^k \binom{N}{k} (N-k)! = \int_0^\infty dt\, e^{-t} (\zeta + t)^N \tag{13}$$

where $\zeta = e^{\beta m \ln N} - 1$, and we have used $\Sigma_{\{S_{i,\tau}\}} S_{i_1,i_1} \ldots S_{i_k,i_k} = (N-k)!$.

In this way for any N we obtain

$$Z = \int \frac{dm}{\sqrt{2\pi/\beta N \ln N}} e^{-\beta N \ln N m^2/2} \int_0^\infty dt\, e^{-t} (t - 1 + N^{\beta m})^N. \tag{14}$$

In the limit $N \to \infty$, Z can be evaluated by taking the saddle point on m and t. The saddle point $m = 0$ always exists and gives $Z = N!$ and $F = -T \ln Z / N \ln N = -T$.

Let us now study the possibility $m \neq 0$. Such a solution exists when the saddle point value of t (that dominates the integral) is such that

$$t < N^{\beta m}. \tag{15}$$

In this case the saddle-point equation for m gives $m = 1$ and (15) reads $t < N^{\beta}$. In the opposite case, $t > N^{\beta}$, the assumption $m \neq 0$ is inconsistent and has to be rejected; so we find that the solution $m = 1$ exists for $T < 1$. The free energy of the $m = 1$ solution is $F = -\frac{1}{2}$ and corresponds to the minimum when $T < \frac{1}{2}$. The free energy of the model as a function of the temperature is given in figure 1. We note the peculiar structure of the model, which in the low-temperature phase is dominated by the ground state and has entropy $S = 0$, and in the high-temperature phase is dominated by the entropy that attains its maximum value $S = N \ln N$, the energy being zero. So in the region $T < 1$, there is coexistence of two phases, one fully correlated with the pattern, the other fully ergodic among the configurations which have zero overlap with the pattern. Exactly the same results would be obtained by taking, instead of permutation matrices, N-states Potts variables. This means that one of the two constraints in (4) is irrelevant. This is a consequence of the fact that we can neglect finite terms with respect to $\ln N$. We think that this still holds in the case of the memorization of p patterns where we will hypothesize it in order to solve the model.

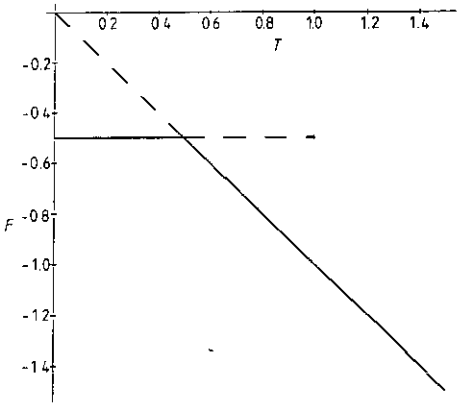

Figure 1. The free energy as a function of the temperature: the full line corresponds to the minimum of the free energy, while the broken lines are the free energies of the metastable states. As explained in the text the solution $m = 0$ exists for all T and minimizes the free energy for $T > \frac{1}{2}$. The solution $m = 1$ exists for $0 \leqslant T \leqslant 1$ and minimizes the free energy for $T < \frac{1}{2}$.

2.2. Memorization of p permutations

In this section we study the memorization of p random permutations. The terminology and the technique we use are borrowed from spin glasses and neural networks theory. In particular we will be interested in the spin glass and the retrieval phases of the system and in the determination of the limit of capacity. We solve the model neglecting one of the constraints (4) of the matrices $S_{i\tau}$, namely the various rows of the $S_{i\tau}$ will

be considered as N-states Potts variables†. This should be a valid approximation provided one can neglect quantities which are finite with respect to ln N. We stress, however, that the validity of this approximation depends on the particular couplings we choose. It is very easy to find examples of coupling matrices for which in a Hamiltonian (6) permutation matrices and Potts variables have a very different ground state and different thermodynamics.

The maximum number of patterns stored in the system is found to scale as $N^3/\ln N$. This scaling can be understood from a simple argument of information theory. The number of 'synapses' in the network is N^4, and the information content per pattern is $\ln N! \sim N \ln N$. Assuming finite information storable per synapse we get the mentioned scaling by just dividing the two numbers. To study the thermodynamical properties of the model in the case of the storing of p patterns, we use the replica trick to average the free energy over the random patterns, following closely the AGS study of the Hopfield model [1, 11]. We will study the retrieval phase with a single condensed overlap and the spin-glass frozen phase (without any condensed overlap).

The thermodynamics of the system has a peculiarity that deserves some attention. Due to the scaling of the entropy as $N \ln N$ we will see that the 'decoupling of the sites' usual in mean-field theories will not lead us to a single-variable partition function, but to a partition function of a system with N possible states, similar to the random energy model [12]. In this way we will find two macroscopic problems nested one into the other that can both lead to a phase transition.

We will assume a single condensed overlap with, say, pattern number one, that can be reduced to $\xi^1_{i\tau} = \delta_{i\tau}$ by a gauge transformation, as explained in the previous section. Indicating with a bar the average over the random patterns we can write

$$\overline{Z^n} = \overline{\sum_{\{S_{i\tau}\}} \exp\left(\beta \frac{\ln N}{2N} \sum_{a=1}^{n} \sum_{\mu=1}^{p} \left(\sum_{i,\tau}^{1,N} S^a_{i\tau} \xi^\mu_{i\tau}\right)^2\right)}$$

$$= \int \prod_a \frac{dm^a}{\sqrt{2\pi/\beta N \ln N}} \exp\left(-\frac{1}{2}\beta N \ln N \sum_a m^{a2} + \beta \ln N \sum_{a,i} m^a S^a_{ii}\right)$$

$$\times \overline{\sum_{\{S_{i\tau}\}} \exp\left(\beta \frac{\ln N}{2N} \sum_a \sum_{\mu>1} \left(\sum_{i,\tau} S^a_{i\tau} \xi^\mu_{i\tau}\right)^2\right)} \tag{16}$$

where m^a is the overlap of the system with pattern one. In appendix A we show how to compute the average over the ξs expanding in series the exponential to the leading order in $N \ln N$. It turns out that terms in β^2, i.e. of the order $P \ln^2 N/N^2$, have to be considered. Re-exponentiating we obtain, to that order,

$$\int \prod_a \frac{dm^a}{\sqrt{2\pi/\beta N \ln N}} \exp\left(-\frac{1}{2}\beta N \ln N \sum_a m^{a2}\right) \Big/ \sum_{\{S_{i\tau}\}} \exp\left(\beta \ln N \sum_{a,i} m^a S^a_{ii}\right.$$

$$\left. + \frac{\alpha\beta^2}{4} \frac{\ln N}{N} \sum_{a,b} \left(\sum_{i,\tau} S^a_{i\tau} S^b_{i\tau}\right)^2 + \frac{9}{8}\alpha\beta^2 \ln N \sum_{a,b} \sum_{i,\tau} S^a_{i\tau} S^b_{i\tau}\right) \tag{17}$$

where we have introduced $\alpha = P \ln N/N^3$, which is kept finite when $N \to \infty$.

Introducing by means of a Hubbard-Stratonovich transformation the usual overlap order parameters $Q_{ab} = (1/N) \sum_{i\tau} \langle S^a_{i\tau} S^b_{i\tau} \rangle$, and evaluating $\overline{Z^n}$ by saddle point on Q_{ab}

† q-states Potts neural networks have been considered in [15-17]. Here we study a different problem where the number of Potts states, N, is equal to the number of units.

and m_a, we get

$$\overline{Z^n} = \text{SP} \exp\left[N \ln N \left(\frac{11}{8}\alpha\beta^2 - \frac{\beta}{2}\sum_a m_a^2 - \frac{1}{2}\alpha\beta^2 \sum_{a<b} Q_{ab}^2 \right) \right]$$

$$\times \sum_{\{S_{i\tau}\}} \exp\left[\ln N \left(\alpha\beta^2 \sum_{a<b} \left(\frac{9}{4} + Q_{ab} \right) \sum_{i,\tau} S_{i\tau}^a S_{i\tau}^b + \beta \sum_{i,a} m_a S_{ii}^a \right) \right]. \tag{18}$$

where SP stands for 'saddle point'. At this point we crucially use the 'Potts hypothesis' and decouple the rows of the matrix $S_{i\tau}$, writing the sum over $\{S_{i\tau}\}$ in $\overline{Z^n}$ as the Nth power of the 'single-site' partition function ζ:

$$\zeta = \sum_{\{S_\tau\}} \exp\left[\ln N \left(\alpha\beta^2 \sum_{a<b} \left(\frac{9}{4} + Q_{ab} \right) \sum_{\tau} S_\tau^a S_\tau^b + \beta \sum_a m_a S_1^a \right) \right]. \tag{19}$$

We notice *en passant* that exactly the same expression would be obtained from a spin-glass Hamiltonian

$$H = -\ln N \left(\sum_{i\tau} S_{i\tau}\delta_{i\tau} \right)^2 - \sum_{i\tau, j\sigma} J_{ij}^{\tau\sigma} S_{i\tau} S_{j\sigma} - \sum_{i\tau} K_{i\tau} S_{i\tau} \tag{20}$$

where $J_{ij}^{\tau\sigma}$ and $K_{i\tau}$ are independent Gaussian variables of zero mean and variances respectively

$$\langle J_{ij}^{\tau\sigma 2} \rangle = \frac{\alpha \ln N}{2N} \qquad \text{and} \qquad \langle K_{i\tau}^2 \rangle = \frac{9}{4}\alpha \ln N. \tag{21}$$

This shows that the spin-glass phase of this problem will be that of a glass of N-states Potts variables. More general choices for the variances of $J_{ij}^{\tau\sigma}$ and $K_{i\tau}$ lead to a phase diagram similar to those we find, and will not be discussed.

As announced, the ζ that comes out from the decoupling of the rows of the matrix $S_{i\tau}$ can be thought as a partition function of a system of N states with an energy of order $\ln N$. As such the decoupled system can still undergo a phase transition. More precisely, in order to find the saddle point of (18), we need to proceed in two steps:

(1) For a fixed set of properly chosen Q_{ab} and m_a (which we shall call external parameters), one must compute the free energy of the reduced problem:

$$n\phi(Q_{ab}, m_a) = -\frac{1}{\beta \ln N} \ln \zeta. \tag{22}$$

(2) One must find the saddle point on Q_{ab}, m_a of the function

$$\frac{11}{8} n\alpha\beta^2 - \frac{\beta}{2}\sum_a m_a^2 - \frac{1}{2}\alpha\beta^2 \sum_{a<b} Q_{ab}^2 - \beta\phi(Q_{ab}, m_a). \tag{23}$$

The unusual problem here is that ϕ itself is not necessarily an analytic function of Q_{ab}, since it is the free energy of a problem which has an infinite number of degrees of freedom (in the $N \to \infty$ limit).

To solve problem 1 we can either use the replica trick, with Parisi's ansatz, or we can assume the Parisi ansatz *only for the external parameters*, continue analytically ϕ to $n = 0$, and evaluate it by a direct probabilistic technique. Let us discuss the computation with replicas. (In appendix B we show how to use the alternative method.)

Introducing the matrix $q_{ab} = \Sigma_\tau S_\tau^a S_\tau^b$, whose elements can take the values zero or one, we can write ζ as

$$\zeta = \sum_{\{q_{ab}\}} \exp\left[\ln N\left(\alpha\beta^2 \sum_{a<b}\left(\frac{9}{4}+Q_{ab}\right)q_{ab}\right)\right]$$
$$\times \sum_{\{S_\tau\}} \exp\left(\ln N\beta m \sum_a S_1^a\right) \prod_{a<b} \delta\left(q_{ab} - \sum_\tau S_\tau^a S_\tau^b\right). \tag{24}$$

The sum over $\{q_{ab}\}$ will be evaluated by the 'saddle point'. We will restrict our variational space to matrices $\{Q_{ab}\}$ and $\{q_{ab}\}$ of the Parisi form [9]. Due to the fact that q_{ab} can only take on values 0 and 1, the most general Parisi ansatz for it is a one-step replica symmetry breaking (RSB) matrix, parametrized in terms of the single breaking parameter y, such that q_{ab} is equal to 1 inside diagonal blocks of side y, and zero outside. The group of replica permutations that leave ζ invariant coincides with the group G of invariance of the matrix Q_{ab}. On the other hand, self-consistently one finds that Q_{ab} is given by the mean over all the different (equivalent by symmetry) saddle points q_{ab}^{SP} of (24)

$$Q_{ab} = \frac{\Sigma_{SP}\, q_{ab}^{SP}}{\Sigma_{SP}\, 1}. \tag{25}$$

It is clear that all the relevant saddle points in (25) differ by a relative permutation of G; so

$$Q_{ab} = \frac{1}{|G|} \sum_{\pi\in G} q_{\pi(a)\pi(b)}. \tag{26}$$

The most general Parisi matrix that can solve the self-consistency equation (26) is two-steps RSB with parameters Q_2, Q_1, Q_0 and x_2, x_1, in standard notations:

$$Q_{ab} = \begin{cases} Q_2 & I(a/x_2) = I(b/x_2) \\ Q_1 & I(a/x_1) = I(b/x_1) \qquad I(a/x_2) \neq I(b/x_2) \\ Q_0 & \text{otherwise.} \end{cases} \tag{27}$$

where $I(x)$ is the integer part of x. However we shall see hereafter that the saddle-point solution is always a 'one-step breaking' matrix with $Q_2 = Q_1$ and $x_2 = x_1 \equiv x$. It is easier to start with such a matrix, and then to show that the most general two-step breaking collapses onto a one-step breaking matrix on the saddle point. Let us thus suppose that Q has a one-step breaking form with parameters Q_1, Q_0, x, and $m_a = m$ for all a. The free energy $\phi(Q_0, Q_1, x)$ of the internal problem can be computed by a saddle-point method on the matrix q_{ab}, that is on the breaking parameter y. This internal problem is actually some elaboration of the random-energy model [12], where one considers non-integer moments of the partition function. Indeed let us go back to (19) and write explicitly ζ for a one-step RSB Q_{ab}:

$$\zeta = \sum_{\{S_\tau^a\}} \exp\left[\left[\ln N\beta m \sum_a S_1^a + \ln N\frac{\alpha\beta^2}{2}\right.\right.$$
$$\left.\left.\times\left\{\left(Q_1+\frac{9}{4}\right) + \sum_{\tau=1}^{N}\left[\left(Q_0+\frac{9}{4}\right)\left(\sum_a S_\tau^a\right)^2 + (Q_1-Q_0)\sum_g\left(\sum_{a\in g} S_\tau^a\right)^2\right]\right\}\right]\right] \tag{28}$$

where the index g (going from 1 to n/x) labels the various blocks of x replicas appearing in the matrix. By a Hubbard-Stratonovich transformation, and performing the sum over the S_τ^a, we get

$$\zeta = \exp\left(\ln N \frac{\alpha\beta^2}{2}\left(Q_1+\frac{9}{4}\right)\right)\int \prod_\tau D\varepsilon_\tau \times\left[\int \prod_\tau D\eta_\tau\left(\exp(\ln N\beta m+\sqrt{\ln N}(\gamma\varepsilon_1+\delta\eta_1))+\sum_{\tau=2}^{N}\exp[\sqrt{\ln N}(\gamma\varepsilon_\tau+\delta\eta_\tau)]\right)^x\right]^{n/x} \tag{29}$$

where $Dy = \exp(-y^2/2)\,dy/\sqrt{2\pi}$ and we have set $\gamma = \sqrt{\alpha\beta^2(\frac{9}{4}+Q_0)}$ and $\delta = \sqrt{\alpha\beta^2(Q_1-Q_0)}$. This representation allows us to derive the results on ϕ without resorting to the replica method, as is shown in appendix B.

Let us consider here the replica point of view. We analyse separately the cases $m \neq 0$ and $m = 0$.

Let us first assume $m \neq 0$. In this case two saddle points in ζ are possible:

(1) $q_{ab} = 1$ for all ab and $\langle \Sigma_\tau S_\tau^a \rangle = 1$ for all a:

$$\zeta_1 = \exp\left(n \ln N\beta m + \ln N\alpha\beta^2 \sum_{a<b}\left(\frac{9}{4}+Q_{ab}\right)\right) \tag{30}$$

(2) q_{ab} is one-step RSB with breaking parameter y; $\langle \Sigma_\tau S_\tau^a \rangle = 0$:

$$\zeta_2 = \exp\left[\ln N\left(\alpha\beta^2 \sum_{a<b}\left(\frac{9}{4}+Q_{ab}\right)q_{ab}+n/y\right)\right] \tag{31}$$

where we have used $\Sigma_{\{S_\tau\}} \prod_{a<b} \delta(q_{ab} - \Sigma_\tau S_\tau^a S_\tau^b) = N^{n/y}$.

If saddle point (1) dominates, the assumption $m \neq 0$ is consistent and leads to

$$m = 1 \qquad Q_{ab} = 1 \quad \forall ab \tag{32}$$

with a free energy

$$F = -\tfrac{1}{2} \tag{33}$$

while if saddle point (2) dominates, the hypothesis $m \neq 0$ is inconsistent. In fact, it would lead to $m = 0$. To determine the range of existence of the solution $m = 1$, we have to study when saddle point (1) dominates, for m and Q_{ab} of the form (32). The saddle point (1) gives for ϕ

$$\phi_1 = -1 + \frac{13\alpha}{8T} \tag{34}$$

while saddle point (2) gives

$$\phi_2 = \min_{0\leq y\leq 1}\left(\frac{1}{y} - \beta^2\alpha\frac{13}{8}(1-y)\right) = \begin{cases} -T & \text{if } \alpha > 8/13T^2 \\ 13\alpha/8T - \sqrt{\frac{13}{2}\alpha} & \text{if } \alpha < 8/13T^2 \end{cases} \tag{35}$$

the saddle point (1) dominates, and consequently the solution $m = 1$ exists for

$$\begin{cases} \alpha < \frac{2}{13} & T < \frac{1}{2} \\ \alpha < \frac{8}{13}T(1-T) & \frac{1}{2} < T < 1 \end{cases} \tag{36}$$

leading to a 'capacity' $\alpha_c = \frac{2}{13}$. Note that differently from other models (e.g. the Hopfield model) here when retrieval is possible, it is always perfect.

As we will see this solution does not correspond in all the region of existence to the absolute minimum of the free energy.

Let us now study the case of no condensed overlap, $m = 0$. Let us write the variational free energy as a function of Q_1, Q_0, x, y:

$$-\beta F = \frac{11}{8}\alpha\beta^2 + \frac{\alpha\beta^2}{4}[Q_1^2(1-x) + Q_0^2 x] - \beta\phi(Q_1, Q_0, x, y) \tag{37}$$

with ϕ given by

$$-\beta\phi = \frac{1}{y} - \frac{9}{8}\alpha\beta^2(1-y) - \frac{\alpha\beta^2}{2}\{\theta(y-x)Q_1(1-y) + \theta(x-y)[Q_1(1-x) + Q_0(x-y)]\}. \tag{38}$$

In this case the order of optimization of the various parameters does not matter. Variations with respect to Q_1, Q_0 lead to

$$Q_1 = \theta(x-y) + \theta(y-x)\frac{1-y}{1-x} \tag{39}$$

$$Q_0 = \theta(x-y)\frac{x-y}{x} \tag{40}$$

that substituted into (37) give

$$-\beta F = \frac{\alpha\beta^2}{4} + \frac{1}{y} + \frac{9}{8}\alpha\beta^2 y - \frac{\alpha\beta^2}{4}\left(\theta(x-y)(1-2y+y^2/x) + \theta(y-x)\frac{(1-y)^2}{1-x}\right). \tag{41}$$

Note that

$$\frac{\partial(-\beta F)}{\partial x}\begin{cases} <0 & y > x \\ >0 & x > y \end{cases} \tag{42}$$

so the minimum is attained in all situations for $y = x$. Further minimization with respect to y gives

$$y = \begin{cases} 1 & \alpha < \frac{8}{11}T^2 \\ \sqrt{\frac{8}{11}(1/\alpha\beta^2)} & \alpha \geqslant \frac{8}{11}T^2 \end{cases} \tag{43}$$

$$F = \begin{cases} -(T + 11\alpha/8T) & \alpha \leqslant \frac{8}{11}T^2 \\ -\sqrt{\frac{11}{2}\alpha} & \alpha > \frac{8}{11}T^2. \end{cases} \tag{44}$$

It is easy to see that the retrieval state is the absolute minimum of F in the region

$$\begin{cases} \alpha < \frac{1}{22} & 0 \leqslant T \leqslant \frac{1}{4} \\ \alpha < \frac{8}{11}T(\frac{1}{2} - T) & \frac{1}{4} \leqslant T \leqslant \frac{1}{2}. \end{cases} \tag{45}$$

Note that for zero temperature, the solution $m = 1$ is the state of minimal free energy for $\alpha < \frac{1}{22}$ and continues to exist as a metastable state for $\alpha < \frac{2}{13}$. The spin-glass phase of the model is a one-step RSB with $Q_{ab} = q_{ab}$ for all ab. This means that for the various indices i of the variables $S_{i\tau}^a$, the replicas are all oriented in the same way, i.e. $\Sigma_\tau \langle S_{i\tau}^a S_{i\tau}^b \rangle$ is zero or 1 independently of i. The structure of the states is similar to that of the REM model. The free energy is dominated by several non-overlapping states (uncorrelated with the $\xi_{i\tau}^\mu$), having zero entropy. The phase diagram of the model is displayed in figure 2.

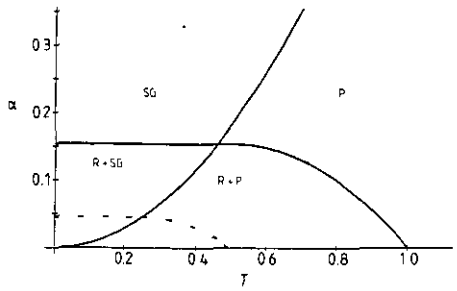

Figure 2. Phase diagram in the plane (α, T). P denotes a paramagnetic phase, SG the spin glass phase, R the retrieval phase. Below the curve that starts at the point $T=0$, $\alpha=\frac{2}{13}=0.154$, the retrieval phase coexists with either the paramagnetic or the spin-glass phase. Below the broken curve the retrieval phase is the global minimum of the free energy.

3. One-dimensional oriented polymers

Consider the one-dimensional problem, in which one maps N different monomers onto a *chain* of N sites i with nearest neighbour interactions:

$$H=-\sum_{i}^{N}\sum_{\tau,\tau'}^{N} S_i^{\tau}S_{i+1}^{\tau'}J_{\tau,\tau'}. \tag{46}$$

Since the pattern ξ_i^{τ} to be stored as a ground state can be taken arbitrarily, let us take

$$\xi_i^{\tau}=\delta_{i\tau}. \tag{47}$$

For the interactions let us choose

$$J_{\tau,\tau'}=\sum_{i}\xi_i^{\tau}\xi_{i+1}^{\tau'}=\delta_{\tau',\tau+1} \tag{48}$$

which differs from the general rule (2) because we consider an *oriented* chain in which the order of the monomers is fixed: the monomer τ at the site i interacts with the monomer $\tau+1$ at the site $i+1$ but it does not interact with the same monomer at the site $i-1$. The reason why we consider this oriented problem will be discussed at the end of this section. The energy corresponds to a certain cost whenever a link between monomers τ and $\tau+1$ is broken, but this cost is independent of the distance between the monomers: the interaction is short-range. A different one-dimensional problem has been studied by Derrida *et al* [14]. The partition function is

$$Z=\sum_{\{S_i^{\tau}\}}\exp\left(\beta\log N\sum_{i,\tau}^{N}S_i^{\tau}S_{i+1}^{\tau+1}\right). \tag{49}$$

The ground-state configuration of the system is obviously the diagonal matrix $S_i^{\tau}=\delta_{i\tau}$. Since the energy (46), is gained due to neighbouring 1s along the diagonal direction, a general way of creating excitations is to produce k 'breaks' among the N lines of the diagonal matrix at lines $m_1,\ldots,m_k$. This breaks the matrix into $k+1$ rectangular blocks of sizes $m_1N,(m_2-m_1)N,\ldots,(N-m_k)N$. Any excited state with energy $k-N$ is obtained by a permutation of the $k+1$ blocks, such that any pair of adjacent blocks is broken (see figure 3).

Therefore the partition function can be written as follows:

$$Z=\sum_{k=0}^{N-1}\exp[\beta(\log N)(N-1-k)]C_{N-1}^{k}P_k \tag{50}$$

$$
\begin{array}{c}
\\
1\\
\\
2\\
\\
\\
\\
3\\
\\
\vdots\\
k
\end{array}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0\\
0 & 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & \dots & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 0 & \dots & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & \dots & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 1
\end{pmatrix}
\Rightarrow
\begin{array}{c}
\\
1\\
\\
\vdots\\
k\\
\\
\\
\\
3\\
\\
2\\
\\
\end{array}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0\\
0 & 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & \dots & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & \dots & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 0 & \dots & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots & 0\\
- & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 1
\end{pmatrix}
$$

Figure 3. An excitation with energy $k-N$. $k+1$ blocks are permuted in such a way that any pair of adjacent blocks is broken.

where $C_N^k = N!/k!(N-k)!$ is the number of positions of k 'breaks' among N lines, and P_k is the number of permutations of $(k+1)$ elements, such that no pair among them remains to be nearest neighbours.

One can easily derive the recursion equation for P_k

$$P_k = (k+1)! - \sum_{l=0}^{k-1} C_k^l P_l \tag{51}$$

where $P_0 \equiv 1$. The solution of the above equation is (appendix C)

$$P_k = k! \sum_{m=0}^{k} \sum_{l=0}^{m} \frac{(-1)^l}{l!} \tag{52}$$

or in the integral form

$$P_k = \int_0^1 \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}x\, t(tx)^k \exp(-tx-1) + \int_0^{\infty} \mathrm{d}t \int_1^{\infty} \mathrm{d}x\, t(tx)^k \exp(-tx-1). \tag{53}$$

Using the above equation for the partition function one gets

$$Z = N^{\beta}\left(\int_0^1 \mathrm{d}t \int_{-1}^{\infty} \mathrm{d}x\, t \exp(-tx-1)(N^{\beta}+tx)^N + \int_0^{\infty} \mathrm{d}t\, t \exp(-t-1)(N^{\beta}+t)^N\right). \tag{54}$$

To leading order in $N \ln N$ this gives

$$\begin{aligned} Z &\simeq \exp(\beta N \log N) \qquad \beta > 1\\ Z &\simeq \exp(N \log N) \qquad \beta < 1. \end{aligned} \tag{55}$$

For the order parameter

$$m = \frac{1}{N} \sum_{i,\tau}^{N} \langle S_i^{\tau} S_{i+1}^{\tau+1} \rangle = \frac{1}{N \log N} \frac{\mathrm{d}}{\mathrm{d}\beta} \log Z \tag{56}$$

one gets

$$m = \begin{cases} 1 & \text{if } T < 1 \\ 0 & \text{if } T > 1. \end{cases} \tag{57}$$

The obtained result shows that the behaviour of the one-dimensional oriented system is similar to that of the infinite-dimensional model with the only difference being that at low temperatures there is only one state in the system which has perfect overlap with the stored pattern, and there is no disordered state. Note also that the problem of storing P patterns in one dimension does not exist. It can be easily checked that there are barrierless transitions between any two arbitrary patterns, and therefore if one stores more than one pattern, the ground state of the system will have equal overlaps with all of these patterns. For the same reason the unoriented one-dimensional chain, in which one changes (48) to $J_{\tau\tau'} = \delta_{\tau',\tau+1} + \delta_{\tau',\tau-1}$ is less interesting: there are two ground-state configurations which are symmetric, and the energy barrier between them is finite (equal to 1).

4. Conclusion

It is strange that the two extreme systems that we have studied (and which are quite different from the initial problem (1), (2)) seem to have very similar properties as far as the retrieval of one pattern is concerned. The main difference of course is that in the one-dimensional model one can store only one pattern, while the maximal number of stored patterns for 'polymers' on the fully connected lattice is $\frac{2}{13}N^3/\ln(N)$. It is not clear to us which features of the solution will remain for a finite-dimensional polymer, where the linear constraint becomes crucial. In view of the above it seems reasonable to conjecture that one should use relatively long-range interactions in order to be able to memorize many shapes.

Perhaps one of the most interesting aspects of this work is the method that has been used to study the statistical mechanics of permutations. We have shown explicitly in one case (the one-pattern case) that one can safely replace the permutation matrices by N-state Potts variables. Even with this replacement the mean-field theory is non-trivial (in the case of the storage of many patterns). The reason is that even a single Potts variable can be in one of N states, and one takes $N \to \infty$. Therefore the Boltzmann sum for one variable in an external field is non-trivial: it already corresponds in some sense to a problem with an infinite number of degrees of freedom, and in particular it can exhibit phase transitions. We think that this is inherent to having as basic configurations the permutations, and this effect could show up in other problems where this is the case.

Appendix A

The average over the patterns

$$\sum_{\xi} \exp\left[\frac{1}{2}\gamma \sum_{a}^{n} \sum_{\mu}^{P} \left(\sum_{i,\tau}^{N} S_{i\tau}^{a} \xi_{i\tau}^{\mu}\right)^2\right] \tag{A1}$$

where $\gamma = (\beta \log N)/N$, can be represented as follows:

$$\left[\left\langle\!\left\langle \exp\left(\frac{1}{2}\gamma \sum_{a}^{n} \sum_{i_1\tau_1} \sum_{i_2\tau_2} S_{i_1\tau_1}^{a} S_{i_2\tau_2}^{a} \xi_{i_1\tau_1} \xi_{i_2\tau_2}\right)\right\rangle\!\right\rangle\right]^{P}. \tag{A2}$$

Here $\langle\langle \ldots \rangle\rangle$ denote the averaging over the matrices $\xi_{i\tau}$. Expanding in powers of $\gamma \ll 1$ one gets the leading contribution

$$\exp\left[\frac{1}{2}P\gamma \sum_{a}^{n} \sum_{1,2} S_1^a S_2^a \langle\langle \xi_1 \xi_2 \rangle\rangle + \frac{1}{8}P\gamma^2 \sum_{a,b}^{n} \sum_{1,2,3,4} S_1^a S_2^a S_3^b S_4^b (\langle\langle \xi_1\xi_2\xi_3\xi_4 \rangle\rangle - \langle\langle \xi_1\xi_2 \rangle\rangle \langle\langle \xi_3\xi_4 \rangle\rangle)\right]. \tag{A3}$$

Here the subscripts $1, \ldots, 4$ stand for $i_1\tau_1, \ldots, i_4\tau_4$.

According to the definition of the matrix $\xi_{i\tau}$ the product of two matrix elements is equal to 1 or 0. If the line and the row numbers of the two elements coincide, then the probability to have 1 is equal to $(N-1)!/N! = 1/N$. If the row and the line numbers of the two elements are different then the probability to have 1 is equal to $(N-2)!/N! = 1/N(N-1)$. Therefore

$$\langle\langle \xi_{i_1\tau_1} \xi_{i_2\tau_2} \rangle\rangle = \frac{1}{N}\delta_{i_1 i_2}\delta_{\tau_1\tau_2} + \frac{1}{N(N-1)}(1-\delta_{i_1 i_2})(1-\delta_{\tau_1\tau_2}). \tag{A4}$$

Since the summation over the indices i and τ will be performed in (3), and we do not need higher order in $1/N$ terms, (4) can be approximated as follows:

$$\langle\langle \xi_1 \xi_2 \rangle\rangle \simeq \frac{1}{N}\delta_{1,2} + \frac{1}{N^2} \tag{A5}$$

(the terms like $(1/N^2)\delta_{1,2}$ are proportional to $1/N$ after summation over indices). Similar combinatorial arguments give

$$\begin{aligned}\langle\langle \xi_1\xi_2\xi_3\xi_4 \rangle\rangle \simeq{}& \frac{1}{N}\delta_{1,2}\delta_{2,3}\delta_{3,4} + \frac{1}{N^2}(\delta_{1,2}\delta_{3,4} + \delta_{1,3}\delta_{2,4} + \delta_{1,4}\delta_{2,3}) \\ &+ \frac{1}{N^2}(\delta_{1,2}\delta_{2,3} + \delta_{1,2}\delta_{2,4} + \delta_{1,3}\delta_{3,4} + \delta_{2,3}\delta_{3,4}) \\ &+ \frac{1}{N^3}(\delta_{1,2} + \delta_{1,3} + \delta_{1,4} + \delta_{2,3} + \delta_{2,4} + \delta_{3,4}) + \frac{1}{N^4}.\end{aligned} \tag{A6}$$

Using (A4) and (A5) one gets for the first term in (A3) a trivial contribution

$$\sum_{a}^{n} \sum_{1,2} S_1^a S_2^a \langle\langle \xi_1 \xi_2 \rangle\rangle = \frac{1}{N}\sum_{a}^{n}\sum_{i\tau}^{N} (S_{i\tau}^a)^2 + \frac{1}{N^2}\sum_{a}^{n}\left(\sum_{i\tau}^{N} S_{i\tau}^a\right)^2 = 2n. \tag{A7a}$$

For the second term one obtains, using (A5) and (A6),

$$\begin{aligned}&\sum_{a,b}^{n} \sum_{1,2,3,4} S_1^a S_2^a S_3^b S_4^b \langle\langle \xi_1\xi_2\xi_3\xi_4 \rangle\rangle - \langle\langle \xi_1\xi_2 \rangle\rangle \langle\langle \xi_3\xi_4 \rangle\rangle \\ &\quad = 9\sum_{a,b}^{n}\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right) + 2\sum_{a,b}^{n}\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right)^2.\end{aligned} \tag{A7b}$$

Therefore, for the average equation (A3) one gets

$$\exp\left\{\frac{1}{8}P\frac{\beta^2 \log^2 N}{N^2}\sum_{a,b}^{n}\left[2\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right)^2 + 9\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right)\right]\right\} \tag{A8}$$

(the constant term coming from (A7) is omitted).

Rescaling $P = \alpha N^3/(\log N)$, one finally obtains

$$\exp\left\{\frac{1}{8}\alpha\beta^2 N \log N \sum_{a,b}^{n}\left[2\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right)^2 + 9\left(\frac{1}{N}\sum_{i\tau}^{N} S_{i\tau}^a S_{i\tau}^b\right)\right]\right\}. \tag{A9}$$

Appendix B

In this appendix we calculate

$$\psi = \int \prod_{\tau} D\varepsilon_{\tau} \frac{1}{x} \ln \left[\int \prod_{\tau} D\eta_{\tau} \left(\exp(\ln N\beta m + \sqrt{\ln N}(\gamma\varepsilon_1 + \delta\eta_1)) + \sum_{\tau>1} \exp[\sqrt{\ln N}(\gamma\varepsilon_{\tau} + \delta\eta_{\tau})] \right)^x \right] \tag{B1}$$

for generical values of γ, δ and x.

We recognize in (4) a structure similar to the REM [12]. For $\delta = 0$ the model is actually a REM, while for $\gamma = 0$ (4) is the average of a REM partition function to a non-integer power x, a problem which has been studied in [13]. Observe that

$$\ln \left[\int \prod_{\tau} D\eta_{\tau} \left(\sum_{\tau} \exp[\sqrt{\ln N}(\gamma\varepsilon_{\tau} - \delta\eta_{\tau})] \right)^x \right] \tag{B2}$$

is self-averaging with in respect to the realization of the $\{\varepsilon_{\tau}\}$ due to the effect of the logarithm. As far as the mean over the $\{\varepsilon_{\tau}\}$ is concerned, only typical configurations contribute (i.e. those having a non-vanishing probability in the limit $N \to \infty$).

The situation is different in respect to the mean of

$$\left(\sum_{\tau} \exp[\sqrt{\ln N}(\gamma\varepsilon_{\tau} + \delta\eta_{\tau})] \right)^x \tag{B3}$$

over the $\{\eta_{\tau}\}$. Clearly if $x \to 0$ the mean is quenched and only typical configurations contribute; conversely if $x = 1$ the mean is annealed and the rare samples are important. In intermediate situations the mean will receive contributions from typical and rare samples. Depending on the values of the parameters one contribution can dominate the other.

(i) The contribution of typical configurations:
We can consider in this case the average over the $\{\eta_{\tau}\}$ quenched as well as that over the $\{\varepsilon_{\tau}\}$. $\gamma\varepsilon_{\tau} + \delta\eta_{\tau}$ can be considered a single quenched Gaussian variable with zero mean and variance $\gamma^2 + \delta^2$. The resulting contribution to ψ is the free energy of a REM at inverse temperature $\sqrt{\gamma^2 + \delta^2}$:

$$\psi_{\text{typical}} = -\sqrt{\gamma^2 + \delta^2}\, F_{\text{REM}}(\sqrt{\gamma^2 + \delta^2}) \tag{B4}$$

where $F_{\text{REM}}(\beta)$ is the free energy of the REM at inverse temperature β

$$-\beta F_{\text{REM}}(\beta) = \begin{cases} 1 + \beta^2/2 & \beta < \sqrt{2} \\ \beta\sqrt{2} & \beta > \sqrt{2}. \end{cases} \tag{B5}$$

(ii) The contribution of the rare configurations:
The rare configurations $\{\eta_{\tau}\}$ that contribute are those for which

$$\eta_M = \max_{\tau} \{\eta_{\tau}\} > \sqrt{2 \ln N} \tag{B6}$$

i.e. the largest of the η_τs is bigger than the value it would attain in a typical configuration†. The probability that a given η_σ will be the maximum η_M of the $N\{\eta_\tau\}$, is

$$\frac{e^{-\eta_M^2/2}}{\sqrt{2\pi}} \prod_{\tau\neq\sigma} \int_{-\infty}^{\eta_M} D\eta_\tau. \tag{B7}$$

Assuming $\eta_\sigma/\sqrt{2\ln N}>1$ it is easy to get to the leading order

$$\frac{e^{-\eta_M^2/2}}{\sqrt{2\pi}}. \tag{B8}$$

The contribution of these configurations is, summing over σ and integrating over η,

$$\langle z^x\rangle_\eta^{\text{rare}} = \sum_\sigma \int d\eta\, P_\sigma(\eta)\, e^{x(\gamma\varepsilon_\sigma+\delta\eta)\sqrt{\ln N}}. \tag{B9}$$

The integration over η_M can be performed by saddle point, giving

$$\eta = x\delta\sqrt{\ln N} \tag{B10}$$

$$\langle z^x\rangle_\eta^{\text{rare}} = e^{\delta^2x^2\ln N/2} \sum_\tau e^{-xy\varepsilon_\tau} = e^{\delta^2x^2\ln N/2} Z_{\text{REM}}(\gamma x). \tag{B11}$$

The quenched average over the $\{\varepsilon_\tau\}$ is easily done, and gives

$$\psi_{\text{rare}} = \frac{\delta^2 x}{2} + \frac{1}{x}[-\gamma x F_{\text{REM}}(\gamma x)]. \tag{B12}$$

It is easy to see that typical configurations dominate ($\psi_{\text{typical}} > \psi_{\text{rare}}$) for

$$\sqrt{\gamma^2+\delta^2} < \frac{\sqrt{2}}{x}. \tag{B13}$$

In that case

$$\psi = \psi_{\text{typical}} = \begin{cases} 1+\dfrac{\gamma^2+\delta^2}{2} & \text{if } \sqrt{\gamma^2+\delta^2} \leqslant \sqrt{2} \\ \sqrt{2(\gamma^2+\delta^2)} & \text{if } \sqrt{2} \leqslant \sqrt{\gamma^2+\delta^2} \leqslant \dfrac{\sqrt{2}}{x}. \end{cases} \tag{B14}$$

In the complementary region of the plane (γ, δ), ψ is dominated by rare samples, giving

$$\psi = \psi_{\text{rare}} = \begin{cases} \dfrac{1}{x} + \dfrac{\gamma^2+\delta^2}{2}x & \text{if } \sqrt{\gamma^2+\delta^2} > \dfrac{\sqrt{2}}{x} \quad \text{and} \quad \gamma < \dfrac{\sqrt{2}}{x} \\ \dfrac{\delta^2}{2}x + \sqrt{2}\gamma & \text{if } \gamma > \dfrac{\sqrt{2}}{x}. \end{cases} \tag{B15}$$

It can be shown that the results coincide with those of the replica method described in the text. The phase diagram is displayed in figure 4.

† It can easily be shown that the maximum between N Gaussian variables $\{x_\tau\}$ verifies $\max\{x_\tau\}/\sqrt{2\ln N} = 1$ with probability 1 for $N\to\infty$.

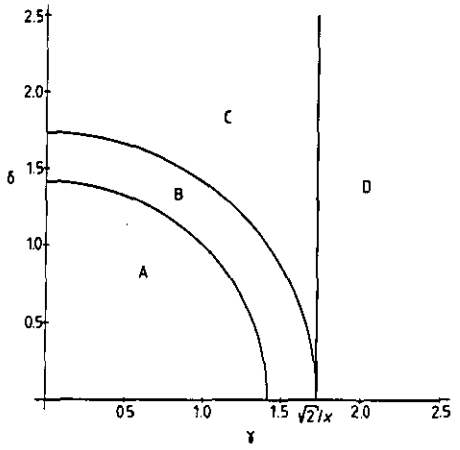

Figure 4. Phase diagram of the model considered in appendix B in the plane (γ, δ). Region A is the high-temperature phase. In region B the free energy is dominated by typical η samples, and the system is frozen. In regions C and D rare η samples dominate.

Appendix C

To solve the equation

$$P_k = (k+1)! - \sum_{l=0}^{k-1} C_k^l P_l \tag{C1}$$

redefine: $P_k = k!\psi_k$. One gets

$$\psi_k = (k+1) - \sum_{l=0}^{k-1} \frac{1}{(k-l)!}\psi_l. \tag{C2}$$

Introducing $\Delta_k = \psi_k - \psi_{k-1}$, from the above equations one obtains

$$\Delta_k = 1 - \sum_{l=0}^{k-1} \frac{1}{(k-l)!}\Delta_l \tag{C3}$$

where $\Delta_0 \equiv 1$, or

$$\sum_{l=0}^{k} \frac{1}{(k-l)!}\Delta_l = 1. \tag{C4}$$

One can easily check that the solution of this equation is

$$\Delta_k = \sum_{l=0}^{k} \frac{(-1)^l}{l!}. \tag{C5}$$

This gives

$$P_k = k! \sum_{m=0}^{k} \sum_{l=0}^{m} \frac{(-1)^l}{l!}. \tag{C6}$$

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