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Eigenstates and limit cycles in the SK model

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Abstract. We study the $T=0$ mean-field equations for infinite-range spin-glass samples of small size by solving exactly the system for different realisations of the coupling constants. We consider both a serial minimisation algorithm, that explores the local minima of the system, and a parallel algorithm, that can also converge to spurious limit-cycle solutions. The cross energy (defined in the paper) plays for the limit cycles the role of the energy for the true solutions, and we then have a way to characterise such spurious solutions (that have been suggested as a possible candidate to the confused state of a realistic memory). In order to substantiate our results, and the large-N extrapolation, we study how some known infinite-N results can be recovered by the knowledge of our small-N results. We also study the basin of attraction of the different kinds of solutions.

Spin-glass models [1, 2] play a very special role at the present time. Not only do they allow us to learn many new things about the statistical mechanics of disordered systems [3-7], but they also allow us to attempt a description of biological models (characterised by their intrinsic complexity; see for example [8-10]). The disordered nature of such models (which makes them interesting) also makes things difficult for us. Metastabilities play a crucial role, and Monte Carlo experiments can very easily be misleading. Here we want to study the behaviour of algorithms used to solve the $T=0$ mean-field equations, which are also exploited in models of a memory. We use a small-N approach [11] by exactly solving small systems (and we look, for example, at dynamical properties of different energy-minimisation algorithms), and we try to extrapolate the results at large N. We will see that this approach is very useful in this case, and that it enables us to learn some crucial new things about the structure of the system and about the dynamics of parallel and serial algorithms.

We will consider an infinite-range spin glass [1, 2]. The N spin variables S_i can take the values $+1$ and -1. In the following N will be not only finite, but also quite small. For $i \neq j$ the coupling constants $J_{i,j}$ (which are random uncorrelated variables) can take the values $+(N-1)^{-1/2}$, $-(N-1)^{-1/2}$ with probability $1/2$, while $J_{i,i}=0$. They are symmetric, i.e. $J_{i,j}=J_{j,i}$, allowing the definition of a Hamiltonian and the use of the usual statistical mechanical formulation. In the large-N limit this choice of the coupling constant is equivalent, as far as thermodynamical quantities are concerned, to the Gaussian one (with mean value 0 and mean-square expectation value $(N-1)^{-1/2}$) and it is very convenient from the computational point of view. We can then define an energy $E=\Sigma\, S_i J_{i,j} S_j$ that is well normalised in the thermodynamical limit. We will express by $\bar{\ }$ the average over the couplings J. We start from the equation

$$S_i' = \operatorname{sgn}\left(\sum_j J_{i,j} S_j\right). \tag{1}$$

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The typical feature of the spin-glass phase (as described by the Parisi solution [4], and as clarified in [5, 6], by the discovery of the ultrametric structure of the phase space) is expressed by the many local minima of the energy. Infinitely high free-energy barriers will separate, in the large-N limit, a very high number of local minima. Local minima with an energy E of the same order of magnitude of the ground-state energy $E^{(0)}$ are stable states in the thermodynamic limit. On the contrary states with $E - E^{(0)} \simeq O(N)$ are metastable states.

We can very easily get a numerical solution of (1) by using a sequential algorithm (see, for example, the discussion in ch 2 of [7]). At each step we flip the selected spin if, by doing that, the energy of the system is lowered. Then we are guaranteed to reach a solution of (1) in a time that is a power in the volume. This solution will be stable against single spin flip, and it will be such that

$$S_i = \mathrm{sgn}\left(\sum_j J_{i,j} S_j\right). \tag{2}$$

We could also try to solve (1) by using a parallel algorithm. We update all of the S_i at the same time, computing, when it is time to update S_j, the energy $S_i J_{i,j} S_j$ by using some 'wrong' old spin S_i (that we already updated, but we did not record yet). Just after a sweep over the whole lattice we inform all the spins of the new situation. We remark (see [8]) that a biological system [9] has somehow an intermediate behaviour between these two intermediate cases. There is surely no clock in order to guarantee synchronisation, but all the neurons of a given domain can fire at the same time. In a parallel-update scheme our initial state can have two kinds of asymptotic behaviour. It can fall in an eigenstate of $J_{i,j}$, like the serial algorithm always does

$$S_i = \mathrm{sgn}\left(\sum_j J_{i,j} S_j\right) \tag{3a}$$

or it can fall in a limit cycle (of length two, for our symmetric case), such that

$$S'_i = \mathrm{sgn}\left(\sum J_{i,j} S_j\right) \qquad S_i = \mathrm{sgn}\left(\sum J_{i,j} S'_j\right). \tag{3b}$$

All the solutions of the serial algorithm are also true solutions of the parallel-updating algorithm (of the form (3a)), since a state stable under single spin flip will also be stable under parallel update (no spin will be flipped at the first update). Then we are sure that the set of solutions (3b) will not contain the true ground state (absolute minimum).

Limit cycles are of some interest, because they could be the representation of a confused memory [10] (indeed one is mainly interested in more complex cases, for example, the one in which the $J_{i,j}$ are asymmetric and long cycles of confusion, perhaps exponential in N, are possible [10]). Their properties are, in this sense, crucial in the determination of what the dynamics governing a realistic memory should be. We will study in the following, for the basic case of the SK model, the mechanism that the updating dynamics uses in order to select such states, and try to understand which is the structure of the basin of attraction of the different kinds of solutions.

Here we approach the problem by solving exactly small samples, and by doing it for many different realisations of the coupling constants $J_{i,j}$. N will be even and it will range from 4 (an easy case, in which we know all the answers *a priori*, and which we used as a check of our programs) to 18. Quenched averages have been taken over 5000 realisations of the uniformly distributed coupling (each $J_{i,j}$ can just take two values), except for the case $N = 18$ where we just solved 1000 systems. For these small

lattice sizes we are able to solve equation (1) for all possible states, by following the evolution of the given state under the effect of the operator $\mathrm{sgn}(J_{i,j}\eta)$. Then we measure, for example, the energies of metastable states, ground states and limit cycles. We also measure quantities such as the number of states that are driven by the evolution law (1) to a eigenstate, to the true ground states or to a limit cycle. We solve (1) both by using a parallel update and by using a serial (no spurious solutions) algorithm. The main advantage of such an approach is that we do not get misled by metastabilities. The problem of diverging relaxation times is very severe in spin glasses, and we want to disentangle the behaviour we are interested in from other (interesting by themselves) effects. It is clear that here we avoid some of the typical risks one takes when using a MC approach, since we analyse the whole phase space of the system. If we can control the large-N limit we will then have acquired a quite precise knowledge of our system. The results of [11], in which small samples were studied mainly in order to understand the behaviour of the order parameter, seem to show that such a control is possible to obtain. We note that when our results can be compared to those [11] they are in good agreement (for example, the ground-state energy as a function of N). We will also see that we match very well the analytic results that are known for large N.

We know [12] that the number of eigenstates of (1) grows as $2^{\alpha_{EV}N}$, with $\alpha_{EV} \simeq 0.287$, i.e. equation (1) has an exponentially growing number of solutions. The maximum number of eigenstates is for $E \simeq -0.506$. The energy of the ground state (as given by the Parisi solution, in agreement with the Monte Carlo data of [2]) is $E^{(0)} \simeq -0.763$. In figure 1 we plot, with the full curve, the energy of the true ground state:

$$E^{(0)} = \overline{S_i^{(0)} J_{i,j} S_j^{(0)}} / N. \tag{4}$$

We agree with [11] in noticing that $E^{(0)}(N)$ is very linear in $N^{-1/2}$. The extrapolation

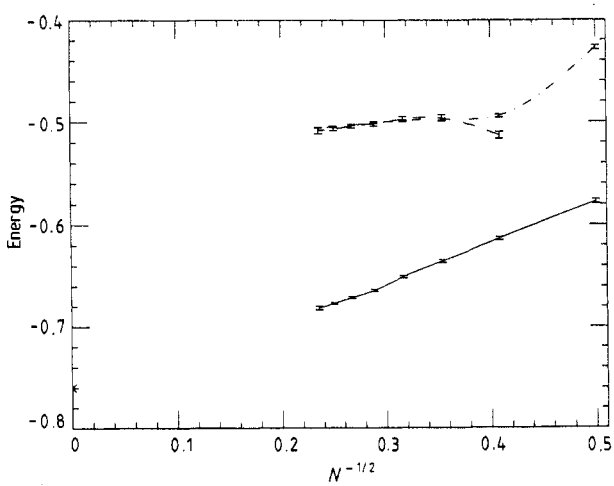

Figure 1. As a function of $N^{-1/2}$ we plot the energy of the true ground state (full curve), the energy of the solutions of the form (3*a*) that are not a global minimum (broken curve), and the expectation value of SJS', where S and S' are the two states of a solution of the kind (3*b*) (chain curve). The states contained in the broken curve are eigenstates different from the true ground state, while those contained in the chain curve are limit cycles (of length two). All the data points are averaged over 5000 J realisations, for which equation (1) has been solved exactly for all the allowed states. The value at $N^{-1/2} = 0$ is the exact result for infinite N, as given by the Parisi solution.

to the correct infinite-N value is indeed very smooth, and the linearity of our data (from $N = 12$–18 at least) impressive.

If replica symmetry were unbroken, one would expect an N^{-1} behaviour. The data confirm previous findings on the power $N^{-1/2}$. This is an interesting result also because the precise origin of the $N^{-1/2}$ corrections is not fully understood at present.

Let us explain what we do in some detail. We solve equation (1) starting from all the 2^N possible states in which the system can be. We consider a state and we start applying the operator $\mathrm{sgn}(J_{i,j}\cdot)$. We do that for both cases of serial and parallel updates. If the state goes, at the first step, in itself (eigenstate) or in a limit cycle (i.e. $\mathrm{sgn}(J_{i,j}S_j) \neq S_i$, $\mathrm{sgn}(J_{i,j}\,\mathrm{sgn}(J_{j,k}S_k)) = S_i$, only for the parallel-updating scheme), we record it as a special state. After enumerating all the *special* states we study them in some more detail. For example, we compute their energies, we select the true ground states, we count them and we measure their energy. For the *normal* states we just record in which special state are they eventually led, in order to understand how the basin of attraction of the system is made.

We are then interested in studying the large-N behaviour of functions of the kind

$$f(N) \simeq 2^{\eta N} \qquad \text{for large } N. \tag{5}$$

We define (since we just study systems with an even number of sites) an N-dependent effective exponent

$$\tilde{\eta}(N) = \log(f(N+2)/f(N))/(2\log 2) \tag{6}$$

where

$$\lim_{N\to\infty} \tilde{\eta}(N) = \eta. \tag{7}$$

The full curve in figure 2 gives the N-dependent exponent $\tilde{\alpha}_{\mathrm{EV}}$, as defined for the number of true solutions (eigenstates) of (1). As we already said this number does

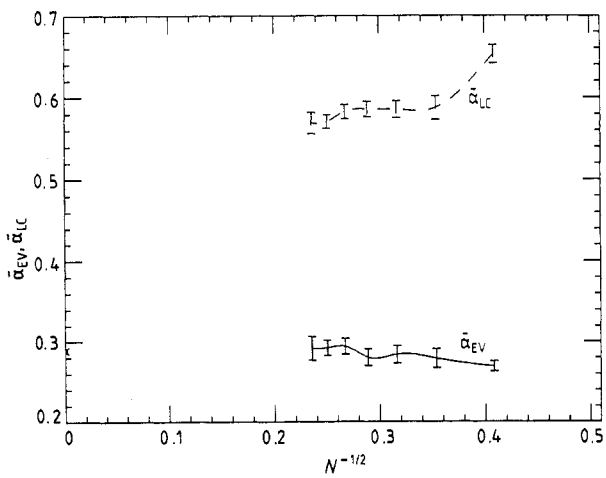

Figure 2. The full curve gives the exponent $\tilde{\alpha}_{\mathrm{EV}}$ of the growth of the number of different eigenstates, as estimated at finite N from the quantity

$$\log(\text{number}(N+2)/\text{number}(N))/2\log 2.$$

The upper (broken) curve is the same quantity $\tilde{\alpha}_{\mathrm{LC}}$ for the number of different limit cycles (3*b*). The value at $N^{-1/2} = 0$ is the exact result for infinite N.

not depend on the algorithm we use, since the true solutions of (1) are stable under serial and parallel updates. The agreement with the known value at $N=\infty$ is very good. The full curves of figures 1 and 2 seem to show that, by using our small-N values, we have a very good control over the infinite-N theory. The exponential growth is already the one we expect in the $N\to\infty$ limit, and we get the correct exponent in a quite unambigous way.

We have seen that the number of eigenstates is growing as known. On the contrary the number of true ground states, figure 3, is very slowly growing (once again, as one expects). Once again it is linear in $N^{-1/2}$, with an extrapolated value, for $N\to\infty$, between 3.5 and 4.

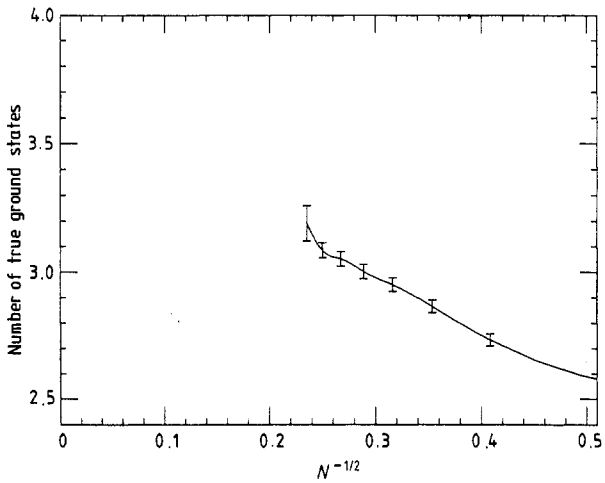

Figure 3. The average number of different global minima as a function of $N^{-1/2}$.

We are ready now to discuss the really interesting features of figure 1. With the broken curve we plot the energy $E^{(EV)}$ of the eigenstates that are not a ground state:

$$E^{(EV)}=\overline{S_i^{(EV)}J_{i,j}S_j^{(EV)}}/N \tag{8}$$

where the $S_i^{(EV)}$ are soltuions of the form (2)-(3a). We eliminate the true ground states in order to get a smoother large-N limit. The true ground states are exponentially suppressed at large N, as we have already discussed and shown, and their energy has quite a large $N^{-1/2}$ dependence on the system size (this dependence is clearly less significant for states of higher energy). But on a small lattice size they are a quite sizeable fraction of the total number of eigenstates. (100% for $N=4$, where we have on average 2.5 eigenstates that are all true ground states. At $N=6$ there are 2.73 ground states and 2.87 eigenstates, while at $N=18$ there are 3.2 ground states compared with 39.5 eigenstates, and our substitution is already quite irrelevant, making a difference of order 3%. The errors on these values are all of the order of 1%.) If we eliminate them the size dependence of our data is very much smoother. We would reach the same conclusions, that we reach here, if we included them in the average (8), but figure 1 would be less impressive.

The chain curve (in the upper part of figure 1 at low N), gives the expectation value

$$E_X^{(LC)}=\overline{S_i^{(LC)}J_{i,j}S_j'^{(LC)}}/N \tag{9}$$

for the spurious solutions (3*b*). This is the equivalent of the energy, but we take the expectation value of $J_{i,j}$ in between the two states of the limit cycle, S and S'. The (quite surprising) agreement between the two curves (already for N values as small as 8) is very good. The crossed expectation value of J for the limit cycles plays the role of the energy for the true solutions. The parallel algorithm is becoming confused about the two possible issues, the one of a small SJS and the one of a small SJS'. It accepts as a good goal a state in which SJS' is as low as $\overline{SJS}$ would be for a typical (low-energy) eigenstate. We have then a manner of discriminating between an eigenstate (a situation in which, in terms of [10], retrieval has been obtained) and a limit cycle (a confused state). We would just have to monitor $\overline{SJS}$ and $\overline{SJS'}$. Let us remark that the numerical evidence for such a claim is quite substantial. The reader can convince himself also by checking that, when using that part of our results which has to converge to known values in the large-N limit, the large-N extrapolation is under good control.

In figure 4 we show that the true energy of a limit cycle solution has nothing special about it. We plot with a full curve

$$E_{\min}^{(\mathrm{LC})} = \overline{\min(S_i^{(\mathrm{LC})} J_{i,j} S_i^{(\mathrm{LC})},\ S_i'^{(\mathrm{LC})} J_{i,j} S_j'^{(\mathrm{LC})})}/N \tag{10}$$

where we take the minimum over the choice of S and S' for each limit cycle, and with the broken curve $E_{\max}^{(\mathrm{LC})}$ defined in the obvious way. The mean value of the two converges to zero, where the density of energy states has its maximum. In figure 5 we plot the expectation value of the difference of the two, showing it is converging to a finite value (of the order of 0.1) in the large-N limit.

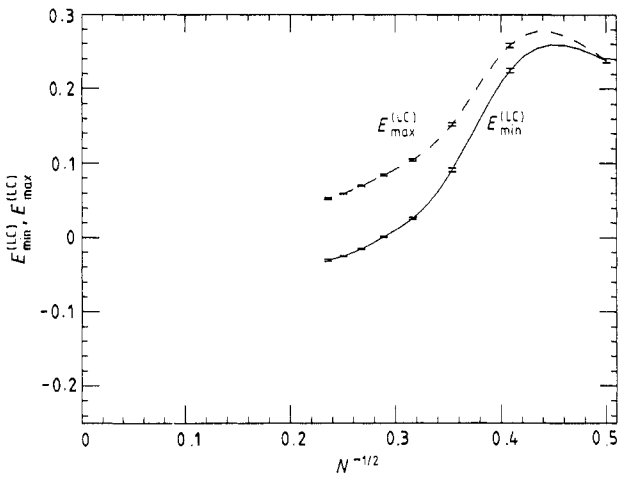

Figure 4. The expectation value of max(SJS, $S'JS'$), where S and S' are the two states of the limit cycle (3*b*) (broken curve) and the expectation value of min(SJS, $S'JS'$) (full curve). This is the true energy of the limit cycles.

We have also computed the cross energy of the lowest-lying limit cycles, i.e. $E_{(\mathrm{LC})}^{(0)\mathrm{X}}$, the equivalent of the ground-state energy for the eigenstate sector. In the absence of replica breaking the difference

$$E^{(0)} - E_{(\mathrm{LC})}^{(0)\mathrm{X}}$$

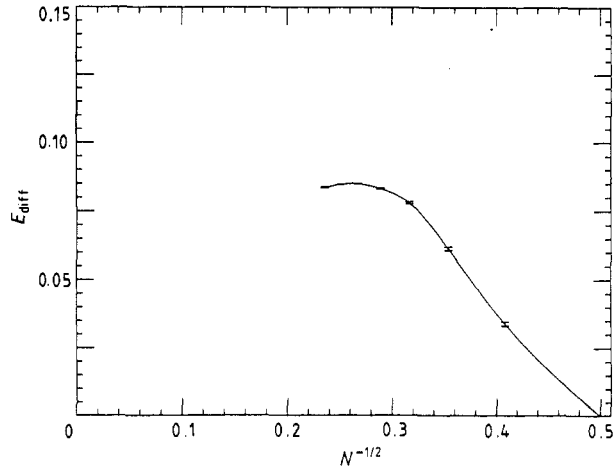

Figure 5. The expectation value of the absolute value of $(SJS - S'JS')$ for solutions of the kind $(3b)$.

is expected to be zero. In figure 6 we plot both $E^{(0)}$ and $E^{(0)X}_{(LC)}$. $E^{(0)}$ extrapolates, as $N \to \infty$, to the correct replica-broken result of -0.76; $E^{(0)X}_{(LC)}$ extrapolates to -0.83, while their average tends to the replica-symmetric value.

Now we are able to discuss the broken curve of figure 2, where we plot $\tilde{\alpha}_{LC}(N)$, the effective exponent of the growth of the number of different limit cycles. We get that roughly

$$\alpha_{LC} \simeq 2\alpha_{EV}. \tag{11}$$

On the basis of our finding about the role of $\overline{SJS'}$ we understand this result quite well. Let us say that there is a number X of states that satisfy the constraint over $\overline{SJS}$ that is needed in order to converge to a true solution of (1). Then if we assume that we reach a confused state when the same constraint applies to $\overline{SJS'}$, we expect to find that X^2 states will be led to limit cycles.

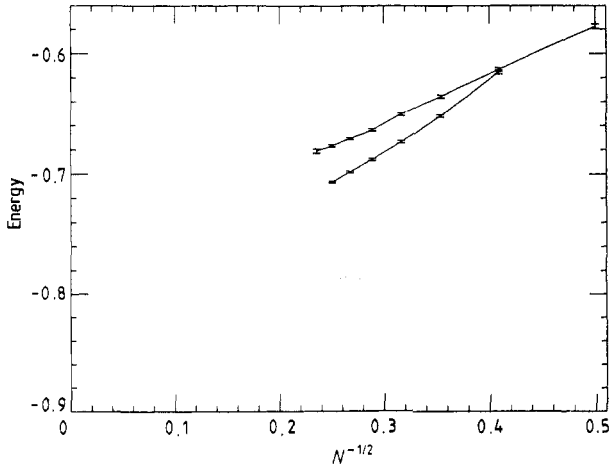

Figure 6. The energy of the true ground states (upper curve), and the cross energy of the lowest-lying limit-cycle states (lower curve).

We have also studied the basin of attraction of the different kinds of solutions. Let us start from the serial (s) case, where all the states are eventually led, under the application of sign $(J_{i,j}\cdot)$, to a true eigenstate. We measure here the number of these states that are going to a true ground state (see figure 7), which we characterise by means of the effective exponent γ_S. We find that $\gamma_S \simeq 0.9$ but the numerical precision we get for the extrapolated value of this number is not very good. In figure 8 we show the same kind of picture for the parallel (P) update. In this case we have three different options, i.e. states going to the true ground state (full curve), states going to an eigenstate (including the true minima, broken curve) and states going to a limit cycle (chain curve).

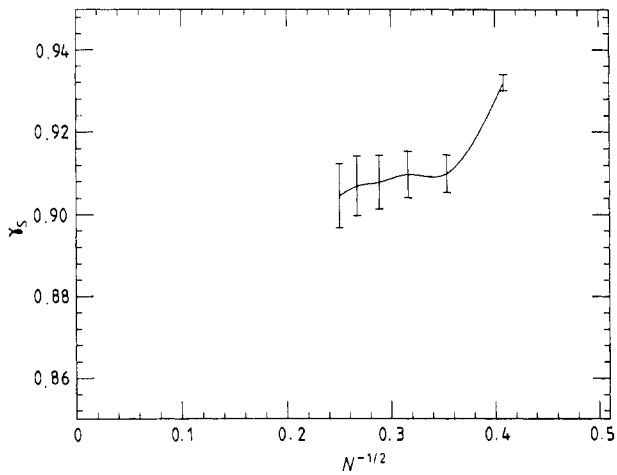

Figure 7. As in figure 2, but for the exponent of the number of states that will fall in the basin of attraction of one of the true ground states, for the serial update. In this case all of the states go to an eigenstate (this is the only possibility).

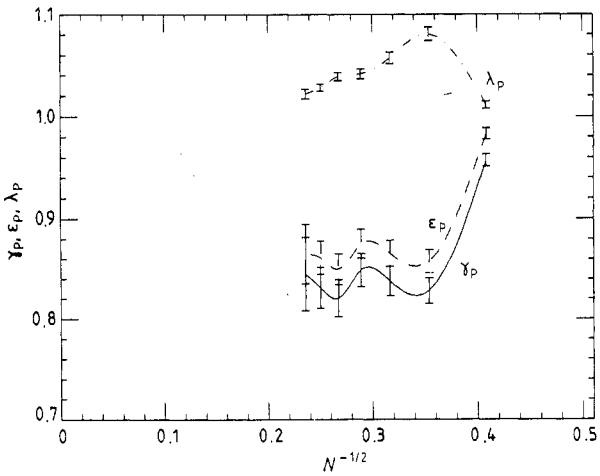

Figure 8. As in figure 7, but using a parallel update. We consider the states that go to the ground state (γ_P, full curve), those that go to an eigenstate (here including the ground state) (ε_P, broken curve), and those that eventually go to a limit cycle (λ_P, chain curve).

As we were expecting, the basin of attraction of the true ground state is exponentially small in N. Indeed a large number of states are, for the N values we consider, in the basin of attraction of the ground state. For the parallel case only an exponentially low number of states are not in the basin of the attraction of the limit cycle. But we notice that at $N = 18$ the 75% of the states that are in the basin of the eigenstates are flowing into a true ground state (262 144 states, of which $229\,017 \pm 967$ are flowing to a limit cycle and $33\,127 \pm 967$ to an eigenstate, and of which $25\,488 \pm 931$ are flowing to a true ground state) as opposed to the fact that only less than 10% of the solutions are true ground states (3.20 ± 7 compared with 39.5 ± 0.6 eigenstate solutions).

We have also studied the fluctuations in the ground-state energy. In figure 9 we plot

$$N \frac{\overline{[(S_i^{(0)} J_{i,j} S_j^{(0)}/N - E^{(0)})^2]}^{1/2}}{E^{(0)}}. \tag{12}$$

This quantity would be asymptotically a constant in a usual random system in non-zero magnetic field (as happens for the free energy of the SK model at sufficiently high temperature). However it has been argued [13] that this quantity should become zero in the large-N limit for the SK model below T_c. Our data (augmented with the data of [14] for N in the range 50-200) suggest that this quantity goes to zero as a power of N. Our best fit gives $N^{-0.222}$ and the data are consistent with $N^{-1/4}$. A theoretical prediction for the exponent is unfortunately lacking.

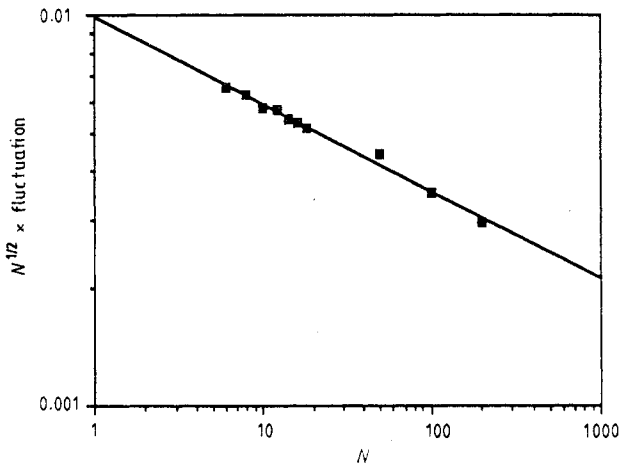

Figure 9. The fluctuation of the energy as defined in (12), plotted against the lattice size N. Our points are in the range $N = 6-18$, while the points of [14] are in the range $N = 50$-200. The straight line is the result of a minimal regression fit.

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