Spin glasses without time-reversal symmetry and the absence of a genuine structural glass transition

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We study the three-spin model and the Ising spin glass in a field using the Migdal-Kadanoff approximation. The flows of the couplings and fields indicate no phase transition, but they show even for the three-spin model a slow crossover to the asymptotic high-temperature behavior for large values of the coupling. We have also evaluated a quantity that is a measure of the degree of non-self-averaging, and we found that it can become large for certain ranges of the parameters and the system sizes. For a spin glass in a field the maximum of non-self-averaging follows a line for given system size that resembles the de Almeida–Thouless line. We conclude that non-self-averaging found in Monte Carlo simulations cannot be taken as evidence for the existence of a low-temperature phase with replica symmetry breaking. Models similar to the three-spin model have been extensively discussed in order to provide a description of structural glasses. Their theory at mean-field level resembles the mode-coupling theory of real glasses. At that level the approach via one-step replica symmetry breaking predicts two transitions, the first transition being dynamic and the second thermodynamic. Our results suggest that in real finite-dimensional glasses there will be no genuine transitions at all, but that some features of mean-field theory could still provide some useful insights.

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I. INTRODUCTION

Despite over two decades of work, the controversy concerning the nature of the ordered phase of short-range Ising spin glasses continues. Monte Carlo simulations of three- and four-dimensional systems appear to be providing evidence for replica symmetry breaking (RSB) in these systems (for recent reviews, see [1,2]). However, recent developments have cast doubt on this interpretation of the Monte Carlo data. In a series of papers on the Ising spin glass within the Migdal-Kadanoff approximation (MKA), we showed that the equilibrium Monte Carlo data in three and four dimensions that had been interpreted in the past as giving evidence for RSB can actually be interpreted quite easily within the droplet picture, with apparent RSB effects being attributed to a crossover between critical behavior and the asymptotic dropletlike behavior for small system sizes [3–7]. We also showed that system sizes well beyond the reach of current simulations would probably be required in order to see dropletlike behavior unambiguously. Very recently, a third view of the nature of the low-temperature phase of spin glasses has emerged. In this picture, there exist droplet excitations on short scales, but on large scales there are system-wide excitations that cost only a finite energy in the thermodynamic limit and have a surface whose fractal dimension is less than the space dimension [8–12]. It remains to be seen whether these excitations survive at larger system sizes. Within the MKA, fractal excitations are not possible, and the signatures of these excitations found in Monte Carlo simulations are therefore not present in the MKA.

There is a close connection between the question of the nature of the spin-glass phase and that of the existence of a phase transition in a spin glass in an external field. Mean-field theory predicts a phase transition to a spin-glass phase with RSB along the so-called de Almeida–Thouless line. The droplet picture predicts no transition. The reason is that in the presence of a field time-reversal symmetry is broken, and there is no symmetry left that could possibly be broken by a phase transition, except for replica symmetry. Monte Carlo simulations of a spin glass in a field [13–15] show some evidence of a phase transition, and in particular of non-self-averaging; however, the situation is complicated by the presence of large finite-size effects due to crossover phenomena. For this reason, Parisi *et al.* [16] studied a different system that also has broken time-reversal symmetry, but is expected not to have strong crossover effects. This system is the three-spin model, where the two-spin products in the Ising spin glass without field are replaced by three-spin products. The numerical evidence for a phase transition in the four-dimensional system seems good, if a quantity that measures the degree of non-self-averaging is studied.

It is the purpose of this paper to study the two mentioned systems without time-reversal symmetry in the MKA, in order to check whether a similar degree of non-self-averaging could be produced by finite-size effects. The flow of the coupling constants shows that for both systems there exists

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only one attractive fixed point, which corresponds to a paramagnet in a random field, and that there is consequently no phase transition within the MKA. Nevertheless, in both systems the coupling constants increase initially for sufficiently low temperatures, indicating that for small system sizes there might be the appearance of a phase transition. Then we looked at the non-self-averaging parameter in both models within the MKA, for various system sizes and parameter values. We found a behavior similar to that reported for the Monte Carlo simulations, and apparent RSB for system sizes similar to theirs. Furthermore, for the spin glass in a field, the maximum of the non-self-averaging parameter as function of the field (for fixed system size) marks a line that can be interpreted as a remnant of the de Almeida–Thouless line.

Some insights into what might be expected in the finite-dimensional three-spin model can be obtained from the mean-field solution of the p-spin model (for a review of which see [17]). It has an analytical solution in the spherical limit which can be obtained by a one-step replica-symmetry-breaking scheme. For our purposes the solution is best understood in terms of metastable states, which can be identified with the solutions of Thouless-Anderson-Palmer (TAP) like equations [18]. The partition function is obtained from the integral

$$Z=\int_{f_{min}}^{f_{max}} df \exp[N\sigma(f)-Nf\beta], \tag{1}$$

where $\beta=1/k_BT$ and N is the number of spins in the system. f is the free energy density of a TAP state. Solutions of the TAP equations exist for $f_{min}<f<f_{max}$, and the number of solutions at free energy density f is exponentially large and given by $\exp[N\sigma(f)]$, with $\sigma(f)$ vanishing at f_{min} and falling discontinuously to zero at f_{max}. For temperatures in the interval $0<T<T_S$ the integral is dominated as $N\to\infty$ by the lower limit of the integral, i.e., states whose free energy Nf differs from the state of lowest energy by only a finite amount. For temperatures in the interval $T_S<T<T_D$ the integral can again be done by steepest descent and is dominated by some value of f lying in the interval $f_{min}<f<f_{max}$. As the temperature approaches T_D this value tends to f_{max}. In the temperature interval $T_S<T<T_D$ an exponentially large number of states contribute to the thermodynamics in contrast to the situation below T_S where only a finite number contribute. Above T_D, only the trivial paramagnetic state contributes. There are thus two phase transitions at mean-field level. The lower-temperature transition at T_S is accompanied by singularities in the free energy but at the higher-temperature transition T_D the free energy is smooth and the presence of a transition is best inferred from singularities in the dynamics.

Now for a finite-dimensional system metastable states with $f>f_{min}$ are unstable. (Imagine in such a state converting a block of spins of linear dimension L to have the orientations that they would have in the lowest state; the free energy gain will be of order L^d; the energy cost of creating such a region will be no more than the cost of breaking all the bonds at the surface of the region, L^{d-1}. Thus the possibility of nucleating lower free energy states prevents the existence of metastable states in finite-dimensional systems.) As the transition at the higher temperature T_D involves the metastable states only, one deduces that it will not exist in a finite-dimensional system. The only transition that could possibly survive to finite dimensions is the one associated with T_S. Our studies, however, indicate that it too probably does not occur in finite-dimensional systems.

Our study of the three-spin model had another, perhaps physically more significant motivation. The three-spin model and its cousins have been extensively studied at mean-field level as models of structural glasses [19]. The higher-temperature transition T_D has a purely dynamic signature (very similar to that in the mode-coupling approach to real glasses [20]), while the transition at the lower temperature T_S is associated with the Kauzmann temperature T_K [21], the temperature at which the configurational entropy of the glass goes to zero. It has been a common belief of many workers for several decades that there is no genuine transition at T_K. Recently this belief has been strongly reinforced by the Monte Carlo simulation of Santen and Krauth [22], who found no evidence of a genuine transition in a simulation in which the particles could be properly equilibrated. Our work strengthens the argument that no genuine transition analogous to T_S or T_K will exist in finite dimensions. Nevertheless, we can see echoes of the mean-field results in our calculations. It is our belief that future work should focus on how the singularities in mean-field results are rounded off in finite dimensions.

This paper is organized as follows. First, we define the models and quantities studied in this paper. Then, we describe the MKA for the two models studied in this paper. We use two different methods in order to make sure that the results do not depend on the particular implementation of the MKA. Next, we study the three-spin model and give our results for the flow of the coupling constants and for the non-self-averaging parameter. In Sec. V, we discuss the spin glass in an external field. Again, we give results for the flows and the degree of non-self-averaging. We also give scaling arguments based on the droplet picture that explain most of our findings. Finally, we summarize and discuss our results.

II. MODELS AND DEFINITIONS

The Edwards-Anderson spin-glass Hamiltonian $\mathcal{H}$ in the presence of a uniform external magnetic field h is given by

$$-\beta\mathcal{H}(\sigma)=\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j+h\sum_i \sigma_i, \tag{2}$$

where the Ising spins σ_i can take the values ±1, and the nearest-neighbor couplings J_{ij} are independent of each other and Gaussian distributed with a standard deviation J. For convenience, the Boltzmann factor β is absorbed into the couplings and fields. Without a field h, the model has a low-temperature phase with nonvanishing correlations $\langle S_iS_j\rangle$ even for spins that are far apart. According to the droplet picture, this phase is unique (up to a global flip of all spins), and it is destroyed as soon as the field is turned on. The reason is that the field induces regions of a sufficiently large radius to flip if the magnetization of this region opposes the field. The radius r of these regions is obtained from the condition that the gain in magnetic energy $hr^{d/2}$ becomes comparable to the loss in coupling energy Jr^{θ}, leading to

$$r \sim (J/h)^{1/(d/2-\theta)}. \tag{3}$$

Here, d is the dimension of the system, and θ the scaling dimension of domain walls. Beyond the radius r, the long-range correlations of the spin-glass phase are destroyed.

In contrast, the RSB picture predicts the existence of infinitely many different phases of comparable free energy in the absence of a field. With increasing field h, the number of phases decreases, and it becomes 1 at the de Almeida–Thouless line $h_c(J)$. At the critical spin-glass transition J_c, the critical field h_c vanishes, and it diverges to infinity as the coupling strength J diverges (i.e., as the temperature goes to zero).

The numerical analysis of the spin glass in a field is hampered by strong crossover effects. Crossover effects are expected to be less strong in the three-spin model, because it has no tunable parameter that can restore time-reversal symmetry and lead to strong crossover effects when small [15]. In the most easily tractable version of this model, each site is occupied by two Ising spins $\sigma_i^{(1)}$ and $\sigma_i^{(2)}$ and the Hamiltonian is given by

$$-\beta\mathcal{H}(\sigma) = \sum_{ij} \left(J_{ij}^{(1)}\sigma_i^{(1)}\sigma_i^{(2)}\sigma_j^{(1)} + J_{ij}^{(2)}\sigma_i^{(1)}\sigma_i^{(2)}\sigma_j^{(2)} + J_{ij}^{(3)}\sigma_i^{(1)}\sigma_j^{(1)}\sigma_j^{(2)} + J_{ij}^{(4)}\sigma_i^{(2)}\sigma_j^{(1)}\sigma_j^{(2)}\right), \tag{4}$$

where ij are nearest-neighbor pairs, and the couplings $J_{ij}^{(n)}$ are chosen independently from a Gaussian distribution with zero mean and width J. When the signs of all spins are reversed, the sign of the Hamiltonian changes also, indicating the violation of time-reversal symmetry.

If finite-dimensional systems have no RSB, this model has no phase transition since there is no symmetry that could be broken. On the other hand, if RSB occurs in finite-dimensional spin glasses, the three-spin model could show a phase transition at some critical coupling strength J_c.

It has proved useful to consider two identical copies (replicas) of the system, with the spins $\{\sigma_i\}$ and $\{\tau_i\}$, and to measure overlaps between them. This gives information about the structure of the low-temperature phase, in particular about the number of pure states. The main quantity studied in this paper is the parameter A, which measures the degree of non-self-averaging, and is defined by

$$A = \frac{[\langle(q-\langle q\rangle)^2\rangle^2]}{[\langle(q-\langle q\rangle)^2\rangle]^2} - 1, \tag{5}$$

where $\langle\cdots\rangle$ and $[\cdots]$ denote the thermodynamic and disorder averages, respectively. The overlap q between the two replicas is given by

$$q = \frac{1}{N}\sum_i \sigma_i\tau_i$$

for the Ising spin glass in a field, and by

$$q = \frac{1}{2N}\sum_i (\sigma_i^{(1)}\tau_i^{(1)} + \sigma_i^{(2)}\tau_i^{(2)})$$

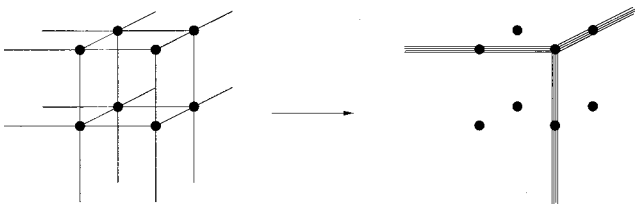

FIG. 1. The Migdal-Kadanoff bond-moving scheme for a cubic lattice.

for the three-spin model. N is the number of sites in the system.

A is most easily evaluated by introducing a coupling between the two replicas, and by differentiating with respect to it. The Hamiltonian for the coupled system is then

$$-\beta\mathcal{H}_\epsilon(\sigma,\tau) = -\beta\mathcal{H}(\sigma) - \beta\mathcal{H}(\tau) + \epsilon N q.$$

The mean overlap is given by the expression

$$\langle q\rangle = \left[\frac{1}{N^2}\frac{\partial}{\partial\epsilon}\ln Z\right]_{\epsilon=0},$$

and its variance by

$$\langle(q-\langle q\rangle)^2\rangle = \left[\frac{1}{N}\frac{\partial^2}{\partial\epsilon^2}\ln Z\right]_{\epsilon=0}.$$

Z is the partition function.

In systems with RSB, the probability distribution $P(q)$ of q is broad, and A has a nonzero limit in the limit of infinite system size. On the other hand, in the absence of RSB, each sample has only one, sample-independent value of q, and A vanishes in the thermodynamic limit. Consequently, an A that increases with increasing system size could be taken as an indicator of RSB. However, we will see in this paper that even systems without RSB can show an increasing A over a wide range of system sizes and parameters.

III. MIGDAL-KADANOFF APPROXIMATION

The Migdal-Kadanoff approximation is a real-space renormalization group that gives approximate recursion relations for the various coupling constants. An exact decimation, which consists in taking the trace over all those spins that do not belong to the coarse-grained lattice, generates higher-order couplings between spins of more that two sites, and is therefore untractable. In order to circumvent this problem, the MKA moves the bonds of a hypercubic lattice before each decimation step in such a way that no higher-order couplings can be generated. If the bond moving is symmetric with respect to the different space directions, one ends up with the scheme represented in Fig. 1.

In a d-dimensional lattice, 2^{d-1} bonds are superimposed as a consequence of bond moving. In the absence of field terms (i.e., of terms that couple only spins that are on the same site i, and are therefore not in a clear way associated with bonds), the 2^{d-1} coupling constants of each of the d bundles of bonds per coarse-grained unit cell simply add up, and the ''naked'' spins that are left behind have no couplings. Taking the trace over the d spins that are on the d

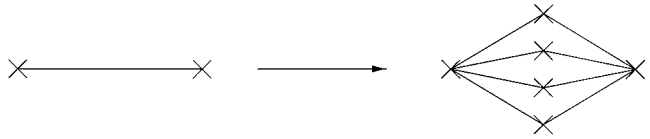

FIG. 2. Construction of a hierarchical lattice.

main bonds leads to coarse-grained coupling constants between neighboring spins on the coarse-grained lattice. Taking the trace over the naked spins gives only a constant contribution to the partition function, which can be neglected. This decimation procedure is iterated n times on a lattice of linear size $L=2^n$, until a single unit cell is left over. Assuming periodic boundary conditions, one can then take the trace over the final spin.

The flow of the coupling constants in this scheme results from alternating the addition of 2^{d-1} bonds with linking two of these new bonds together and taking the trace over the middle spin. Essentially the same flow results when a decimation is done on a hierarchical lattice that is constructed iteratively by replacing each bond by 2^d bonds, as indicated in Fig. 2. The total number of bonds after n iterations is 2^{dn}. Spin decimation on such a lattice is done by taking the trace over the spins that are highest on this hierarchy (i.e., that were added last during the construction procedure). At each decimation step, first the trace is taken over the middle spin of two linked bonds, and then 2^{d-1} bonds are added together to form a new bond, until the lowest level is reached and the trace over the remaining two spins is calculated [23]. Apart from the fact that the order of bond adding and decimation is reversed, the recursion relations for the coupling constants are obtained by the same procedure as for the bond-moving algorithm.

This equivalence between a bond-moving procedure for a hypercubic lattice and a hierarchical lattice no longer holds when field terms are present. In both of our models, these field terms are either present from the beginning (Ising spin glass in a field), or they are initially absent, but are generated during the decimation procedure (three-spin model). For the bond-moving procedure, one has to decide whether the fields will also be moved (and to where), or whether they will remain at their sites, or whether part of them will be moved. This creates a certain freedom in the renormalization scheme, and the most plausible choice is determined by the requirement that the flows of the fields near the zero-temperature fixed point and at the infinite-temperature fixed point shall be those of the hypercubic lattice. However, if the main results of the MKA are to be generic, they should not depend on the precise implementation of the bond-moving algorithm. Otherwise one might doubt that the MKA reflects the features of the real system. For this reason, we have performed the MKA for a variety of different implementations, and we found our main conclusions concerning A to be independent of the implementation. In the following sections, we will give our results for the hierarchical lattice and for a bond-moving scheme that has the correct flow of the field terms.

The treatment of a hierarchical lattice in the presence of field terms is straightforward. In order to understand that the flows of the fields are different on a hierarchical lattice compared to a hypercubic lattice, let us consider a situation where the flows of the couplings go to zero with increasing iteration number, which is the situation that we will encounter below for both models. As long as the couplings are nonzero, each decimation step generates a contribution to the fields at the sites that are left over. The two corner spins, which are left over until the end, consequently receive $2^{n(d-1)}$ field contributions from the first decimation, $2^{(n-1)(d-1)}$ from the second iteration, and so on, until the couplings are virtually zero. For twice the system size, i.e., for a lattice with $n+1$ levels, the mean of the field contribution to the corner spins due to decimations is larger by a factor $2^{(d-1)}$, and so is the variance of the field contribution. Even though the couplings go to zero after a certain number of iterations, the fields keep growing.

In contrast, on a hypercubic lattice, the fields must remain constant as soon as the couplings have become zero. Clearly, this can be achieved only if field terms are not moved to the sites that will not be traced over. On the other hand, field terms must not be left with the ''naked'' spins. The reason is that, near the zero-temperature fixed point where the couplings are very large, all fields must add up under renormalization. Fields must therefore always stay with spins that are coupled to other spins. For this reason, fields should be moved to those d sites that are at the middle of the main bonds. Even with this restriction, there remains some freedom in choosing which field should be moved where. In our simulations, we treated field terms as belonging to bonds. The initial fields were evenly distributed between the ends of all bonds, and the fields generated during decimations naturally ended up at the ends of bonds. When a bond was moved, we moved all its field terms to that end that was to be traced over next.

For the Ising spin glass in a field, the recursion of four different parameters must be considered when studying the flow diagram and thermodynamic quantities. These are the two-spin coupling, the two fields on the two ends of a bond, and a constant. If one evaluates quantities related to the overlap between two replicas, each site has two spins, leading to 16 parameters. The same number of parameters occurs for the three-spin model, if only one replica is needed, as, e.g., for the flows and the phase diagram. For the evaluation of A, we need two replicas, leading to 256 couplings. Luckily, the decimation step can treat all 256 parameters with the same formula, which involves a 256×256 matrix that is calculated once at the beginning of the program.

IV. THREE-SPIN MODEL

This model was studied using Monte Carlo simulations in four dimensions in [15,23,16], and evidence for RSB was found. The authors of [23,16] found in particular that the non-self-averaging parameter A is small for large temperatures, and becomes large for smaller temperatures. Curves for different system size $L=3,4,5,6$ cross at nearly the same temperature, and below this temperature A increases with increasing L. Thus, the degree of non-self-averaging increases with the system size, just as can be expected for a replica-symmetry-breaking transition. Monte Carlo simulations [15,24,16] are usually done with couplings $J=\pm1$. The precise distribution of the couplings, however, should not affect the universality class.

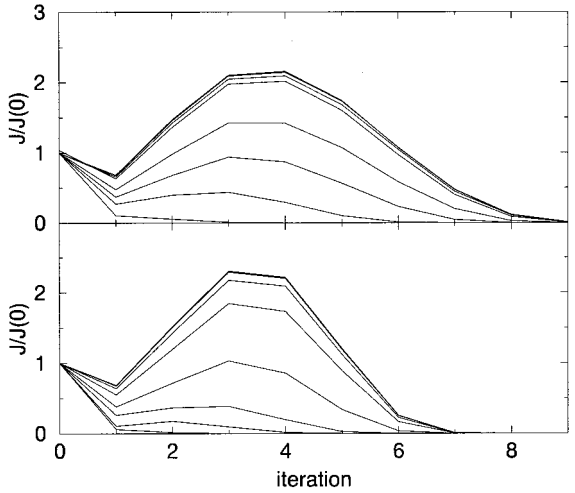

FIG. 3. Flow of the three-spin coupling strength J for bond moving (top) and the hierarchical lattice (bottom) for $d=4$, divided by the initial coupling strength. The curves correspond to $J(0)=0.065,0.13,0.18,0.26,0.5552,1,2,5$ (bond moving) and $J(0)=0.13,0.26,0.35,0.52,1,2,5,10$ (hierarchical lattice) from bottom to top.

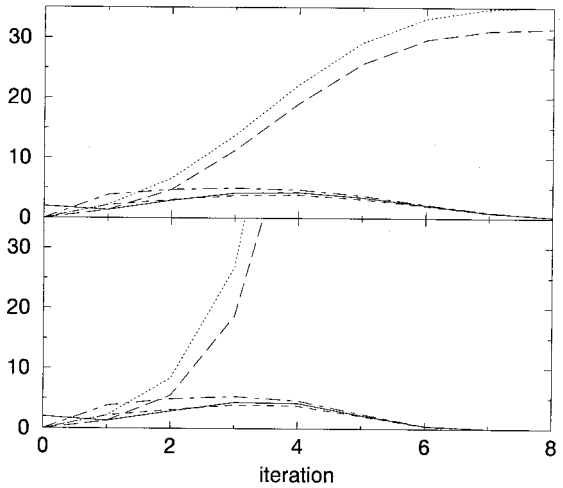

FIG. 4. Flow of the width of the field (long dashed), of the on-site two-spin coupling (dotted), the two-spin coupling across a link (dashed), the three-spin coupling (solid), and the four-spin coupling (dot-dashed) for bond moving (top) and on the hierarchical lattice (bottom) for $d=4$, for an initial three-spin coupling $J(0)=2$.

Analytical results were obtained for the p-spin model in mean-field theory, where one-step RSB was found. This means that the ground state has a nonzero probability of being occupied below a critical temperature T_S (see Sec. I). This mean-field scenario is fundamentally different from the full RSB claimed to be seen in Monte Carlo simulations of the four-dimensional system. Thus, the argument usually employed for spin glasses that mean-field like behavior can be found in finite-dimensional short-range systems fails here.

In the following, we show using the MKA that the assumption of the absence of crossover effects in this model is incorrect, and that A might at low temperatures and for small system sizes increase with increasing system size even if the system is self-averaging in the thermodynamic limit. We mainly focus on the case of four dimensions, but report also some results in $d=2$ and 3. Let us first discuss the flow of the coupling constants as the system is renormalized. Because each bond is connected to four spins, the flow of 16 coupling constants has to be considered. In order to obtain this flow, we iterated the recursion relation on a set of 10^6 bonds. At each iteration, each of the new set of 10^6 bonds was generated by randomly choosing 2^d bonds from the old set. For a hierarchical lattice, where the generated fields remain at that end of a bond at which they are generated, we first took the trace over the inner spins of each of the 2^{d-1} pairs of bonds, and than we added the resulting bonds; for the bond-moving procedure described in the previous section, we first generated two bunches of 2^{d-1} bonds each, then moved the fields of all but the ''original'' bond of each bunch to the inner spin, and took the trace over the inner spin. Figure 3 shows the flow of the width of the three-spin couplings for different initial widths in four dimensions, for the two different algorithms.

One can see that for weak coupling (or, equivalently, high temperature) the coupling strength decreases quickly with increasing system size. However, for stronger coupling or lower temperatures, the coupling strength increases during the first few iterations, and decreases afterward toward its fixed-point value zero, implying that there exists no low-temperature phase with long-range order. The maximum is reached between the third and fourth iterations, or between $L=8$ and $L=16$. For sufficiently strong coupling, the curves reach an asymptotic shape. On the hierarchical lattice, where the fields grow without bounds, the three-spin couplings decrease to zero faster than with bond moving. Furthermore, the curves for the hierarchical lattice seem to correspond roughly to those of the bond-moving procedure if the three-spin couplings are divided by a number around 3. The reason is that the first step during the bond-moving procedure summarizes 8 bonds in one new bond. The width of the three-spin coupling is therefore increased by a factor of $\sqrt{8}$ in four dimensions. In order to compare to the hierarchical lattice or to Monte Carlo simulations on a hypercubic lattice, one should divide the coupling strength of the bond-moving procedure by $\sqrt{8}$.

If one considered only systems of sizes up to 8, one would get the illusion of a phase transition with $(1/J)_c$ around 3 or 4, a value that is not far from the one given for T_c in [16]. (Note that these authors kept the coupling strength fixed at ± 1, and varied the temperature. Their T corresponds therefore to our $1/J$.)

Figure 4 shows the flow of the widths of the different coupling constants for an initial width of the three-spin coupling $J=2$. One can see that the strengths of the field and of the on-site two-spin coupling (which can also be viewed as a ''field'') increase rapidly and without limits for the hierarchical lattice, and that they saturate at a finite value in the bond-moving case. The two-, three-, and four-spin couplings increase during the first few iterations, and then decrease again. Thus, our three-spin model corresponds on large scales to a system with only random fields and random couplings between the σ and τ spins on the same site. There are no couplings between spins on different sites on large enough scales, but sites are independent of each other. Only

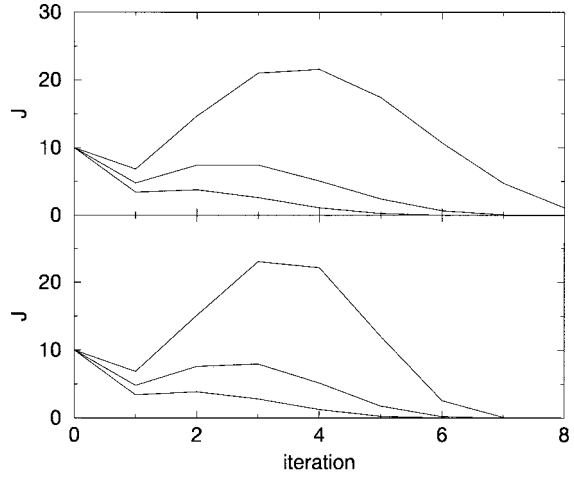

FIG. 5. Flow of the three-spin coupling for an initial value $J(0)=10$ in $d=2,3,4$ dimensions (from bottom to top). The top graph is for bond moving, the bottom graph for a hierarchical lattice.

on small scales could one get the impression that the system has long-range correlations. However, these system sizes are exactly the ones studied in [15,23,16].

The crossover regime becomes larger with increasing dimension. Figure 5 shows the flow of the three-spin coupling for an initial value $J=10$ in $d=2,3,4$ dimensions. Clearly, the strength of the increase and the range of system sizes over which this increase occurs increases with increasing dimension. One can therefore expect that in even higher dimensions the apparent phase transition will become more pronounced.

Next, let us study the non-self-averaging parameter A. As explained in the previous section, A can be evaluated by introducing a coupling between two identical replicas of the system. Since there are now eight spins associated with each bond, the number of couplings that have to be evaluated in the MKA approximation is $2^8=256$. Figure 6 shows A as a function of the coupling strength for different system sizes up to 16, in four dimensions. Larger system sizes could not be studied due to limitations in computer time. One can see that A increases with increasing system size wherever it is appreciably different from zero, and reaches large values. This figure gives the impression that the system shows non-self-averaging. Of course, for larger system sizes, A must eventually decrease again since we know from the flows of the couplings that there is self-averaging in the thermodynamic limit. In contrast to the Monte Carlo simulation results [23,16], our curves for A do not intersect at a coupling strength and A value of the order 1. This may be due to a qualitative difference between the MKA approximation and Monte Carlo simulations, or to the much larger spacing of L values imposed by the decimation procedure.

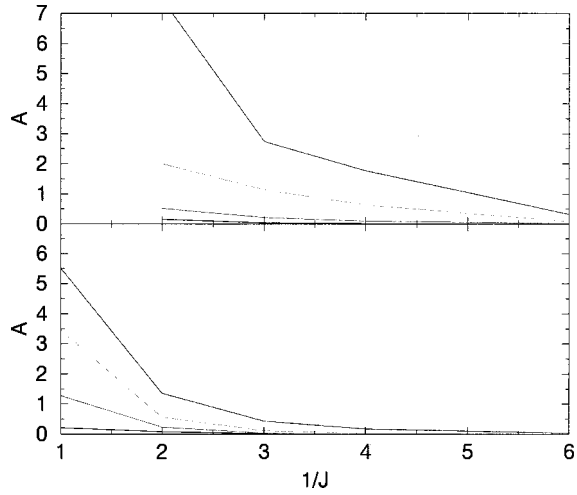

FIG. 6. The non-self-averaging parameter A for $L=2,4,8,16$ (from bottom to top), and $d=4$. The average is taken over 10 000 samples for the smallest system size and 200 samples for the largest. The top graph is again for bond moving and the bottom graph on the hierarchical lattice.

We have performed a similar simulation in $d=2$ dimensions and found that A increases as the system size increases over the range $L=2,4,8,16$. However, for $L=32$ and $L=64$, A decreases. If we assume that the system size for which A is largest increases with each dimension by a factor 2, as it does for the flow of the couplings, we can expect that in $d=4$ the system size for which a decrease in A can be seen is beyond $L=64$.

To summarize this section, we have shown that the three-spin model, even in situations where we know that it self-averages in the thermodynamic limit, can show indications of non-self-averaging at those system sizes typically studied in simulations. Evidence for non-self-averaging found in Monte Carlo simulations must therefore be taken with caution as it might be misleading.

V. ISING SPIN GLASS IN A MAGNETIC FIELD

Monte Carlo simulations in four dimensions show some indication of RSB [13–15]. Just as for the three-spin model and for the spin glass without external field, these findings may again be due to finite-size effects and to the closeness to the critical temperature. Indeed, an investigation of the ground-state structure of a spin glass in a magnetic field [25] shows no indication of RSB. (See, however, the discussion in [26,27].)

In order to test for finite-size effects, we studied the spin glass in a field using the MKA, and determined the non-self-averaging parameter A as a function of the system parameters. We found that the degree of non-self-averaging can be large for the system sizes typically used in simulations, in particular when the contribution of the field to the free energy is comparable to that of the couplings. While most published Monte Carlo simulations were done in four dimensions, we chose to study the MKA in three dimensions, in order to be able to go to larger system sizes. Because there are three parameters to be varied (the system size, the field, and the two-spin couplings), many data points had to be collected, and this is done faster in three dimensions. Of course, we expect that the results of the MKA are similar in four dimensions, if the exponents for three dimensions are replaced with those for four dimensions. Just as for the three-spin model, the apparent non-self-averaging should become even stronger in four dimensions.

First, let us study the flows of the couplings and fields. The decimation procedure leads to the creation of random

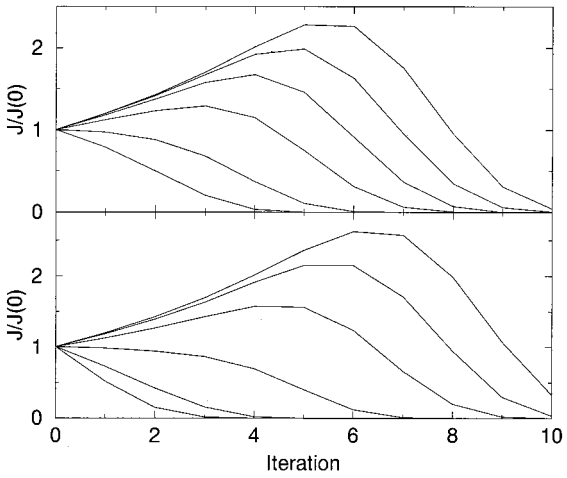

FIG. 7. Flow of the two-spin coupling strength J, divided by the initial strength, for bond moving (top) and the hierarchical lattice (bottom) for $d=3$ and $h=0.1$. The curves correspond to $J(0)=0.3,0.5,1,2,4,8$ from bottom to top, for both graphs. The data were obtained from a set of 50 000 bonds.

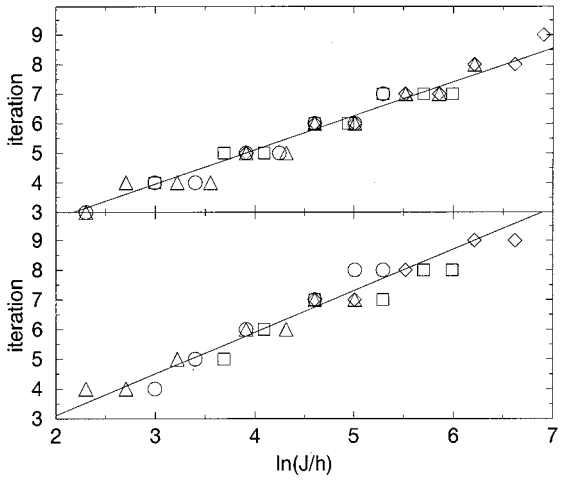

FIG. 8. Iteration number for which the two-spin coupling J reaches its maximum, as a function of $\ln(J/h)$, for different values of h. The symbols stand for $h=0.2$ (triangle), $h=0.1$ (circle), $h=0.05$ (square), and $h=0.02$ (diamond). The lines have the slope 1.15 and offset $C=0.5$ (bond moving, top graph), and slope 1.4 and offset $C=0.3$ (hierarchical lattice, bottom graph).

fields, while the mean value of the field is not changed. Figure 7 shows the flow of the two-spin coupling J for various initial values, and for a fixed field $h=0.1$. For initial couplings smaller than the critical coupling (1.13 for the hierarchical lattice and 0.55 for bond moving), the coupling strength decreases immediately. However, if the initial coupling strength is sufficiently deep in the low-temperature phase, it increases first, until the random field has become strong enough to have a reducing effect on the coupling strength. Ultimately, the flow goes to a fixed point where the coupling strength is zero. On the hierarchical lattice, the width of the field keeps growing indefinitely, while it saturates in the bond-moving case, as discussed in Sec. III. Clearly, there is no phase transition in the presence of an external field, but there are strong crossover effectsif the field is small.

As mentioned in Sec. II, the droplet picture predicts that beyond a length scale $r\sim(J/h)^{1/(d/2-\theta)}$ the contributions of the field and of the couplings to the free energy become comparable, and we expect that the strength of the couplings will decrease beyond this scale. In order to test this prediction, we have plotted in Fig. 8 the iteration number for which the two-spin coupling is largest versus the logarithm of J/h. It should follow the law

$$\log_2 L=\frac{1}{\ln 2[(d/2)-\theta]}\ln(J/h)+C\simeq 1.15\ln(J/h)+C,$$

with a suitable constant C. As the figure shows, the data for bond moving agree nicely with this prediction. For the hierarchical lattice, the slope is larger and has a value around 1.4. This might be due to the fact that the field increases faster on the hierarchical lattice, leading to an earlier reduction in the coupling strength than predicted by the scaling theory.

Next, let us discuss the quantity A, which is a measure of the degree of non-self-averaging. Figure 9 shows our results in the absence of a magnetic field. In the high-temperature phase as well as in the spin-glass phase A decreases with increasing system size and approaches zero, just as one would expect in the absence of RSB. At the critical coupling strength J_c, A remains constant with increasing system size, its value being $A\simeq 0.13$ for the hierarchical lattice and $A\simeq 0.15$ for bond moving. The constancy of A at the critical point can be explained from the scaling behavior of the overlap distribution function $P(q)$. Critical scaling implies

$$[P(q)]=L^{-\beta/\nu}[\tilde{P}(qL^{\beta/\nu})]$$

and

$$[P(q)P(q')]=L^{-2\beta/\nu}[\tilde{P}(qL^{\beta/\nu})\tilde{P}(q'L^{\beta/\nu})],$$

with β being the order parameter critical exponent, and ν the correlation length exponent. Introducing the variable $y=qL^{\beta/\nu}$, we then obtain

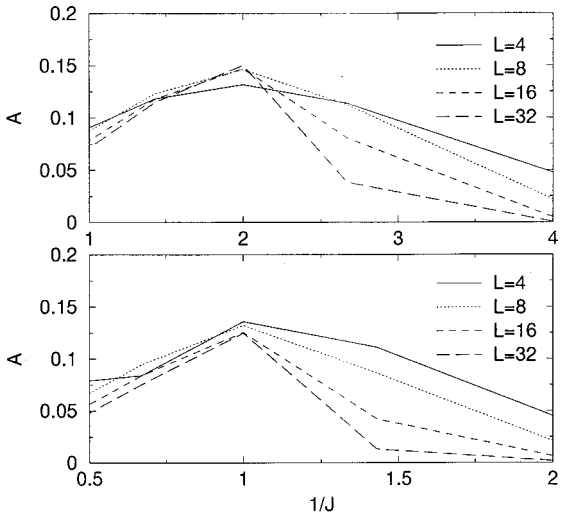

FIG. 9. A as a function of $1/J$ for $h=0$ and $L=4,8,16,32$. The top graph is for bond moving, the bottom graph on a hierarchical lattice.

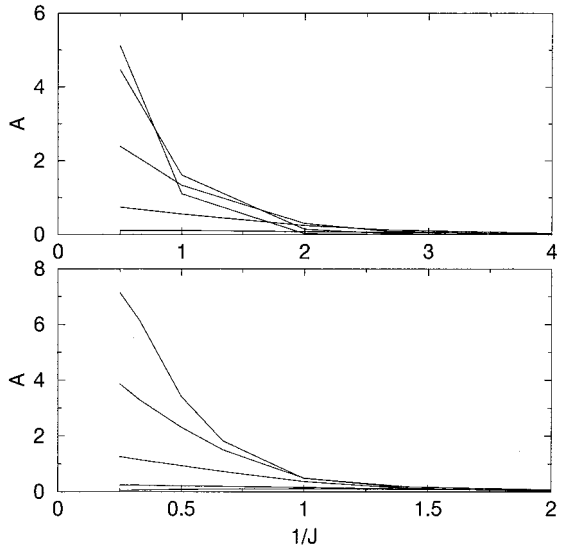

FIG. 10. A as a function of $1/J$ for $h=0.2$ and $L=2,4,8,16,32$ (from bottom to top for the $1/J=0.5$ points), averaged over 2000–50 000 samples. The top graph is for bond moving, the bottom graph for a hierarchical lattice.

$$A=\frac{\int\int y^2 y'^2 \tilde{P}(y)\tilde{P}(y')dydy'}{\left(\int y^2\tilde{P}(y)dy\right)^2}-1$$

independently of L.

For low temperatures $T=1/J$, A seems to follow the law $A\sim TL^{-\theta}$ with $\theta\simeq 0.24$. This can be derived by the following argument. At low temperatures, most samples have a value of $\langle q^2\rangle$ close to 1, and only a fraction p proportional to $kTL^{-\theta}$ of all samples have system-wide excitations and have therefore some other value $\langle q^2\rangle=x<1$. We therefore obtain

$$[\langle q^2\rangle]\simeq 1-p+p[x]$$

and

$$[\langle q^2\rangle^2]\simeq 1-p+p[x^2],$$

leading to

$$A\simeq p(1+[x^2]-2[x])\sim kTL^{-\theta}.$$

In the presence of a magnetic field, we expect A to decrease to zero always for large system sizes, because the system is always in the high-temperature phase without long-range correlations. However, as we will show in the following, A can nevertheless become very large for certain combinations of the system size, the field, and the two-spin coupling strength. One can therefore easily get the impression that the system is not self-averaging, while in reality A increases over only a limited range of system sizes or parameters.

Figure 10 shows our results for A with a magnetic field $h=0.2$. For $J>J_c$, the values are larger than without field, and they increase with increasing system size and decreasing temperature. We expect that as the system size increases further, A will reach a maximum and then decrease again. For fields stronger than $h=0.5$, we see this reversal in the trend of A already for the system sizes studied in the simulations. For $J<J_c$, Fig. 10 shows that the curves for different L intersect each other, such that for high temperatures self-averaging is better for larger system sizes. Thus, the behavior of A for weak fields seems to be qualitatively similar to that of the three-spin model.

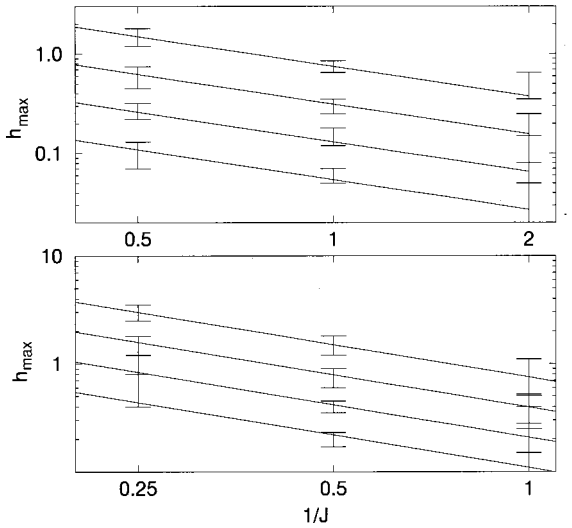

FIG. 11. The field value h_{max} for which A is largest, for $L=4,8,16,32$ (from top to bottom). The straight lines are power laws $h_{max}\propto JL^{-1.26}$ (top graph, bond moving) and $h_{max}\propto JL^{-0.93}$ (bottom graph, hierarchical lattice).

For given system size and coupling strength $J>J_c$, there exists always a value of h for which A has a maximum. This maximum is higher for larger system sizes and for lower temperatures $1/J$. Figure 11 shows the field for which A is largest as a function of $1/J$. The data are in good agreement with a dependence $h_{max}\propto J$ and $h_{max}\propto L^{-1.26}$ for bond moving. This means that A is largest when $h\sim JL^{(d/2-\theta)}$. For the hierarchical lattice, the fit to the data is best for a dependence $h_{max}\propto J$ and $h_{max}\propto L^{-0.93}$. Just as in Fig. 8, the effective value of $d/2-\theta$ appears to be larger on the hierarchical lattice than for bond moving. We suspect that this is due to the fact that the field grows indefinitely on the hierarchical lattice.

These results can be understood if one considers the effect of the field on the overlap distribution $P(q)$. Without field, $P(q)$ is a symmetric function, and varies considerably in shape for different samples for the system sizes typically used in simulations. This feature is seen in Monte Carlo simulations [28] as well as in the MKA [3]. A magnetic field changes the shape of $P(q)$ and moves the weight more and more toward positive q. In the limit $h\to\infty$, all spins are aligned with the field, leading to $P(q)=\delta(1)$. Along the boundary line $L\sim(J/h)^{1/(d/2-\theta)}$, where the field is not yet strong enough to destroy all features of the low-temperature phase, we can expect that at least some samples still have large droplets than can be flipped without much free energy cost. In Monte Carlo simulations [14], one finds indeed for certain intermediate parameter values a $[P(q)]$ that has a pronounced peak at some large q value, and a long and thin tail that extends almost all the way down to $q=-1$. The authors point out that this feature results from most samples

having only the main peak, and other samples having an additional second peak for some other value of q. They go on to argue that this is a non-self-averaging feature characteristic of RSB, and that it would not be expected if there was no RSB. However, they also admit that their simulations do not show a second peak in $[P(q)]$ at a value q_{min}, which is expected from mean-field theory. Although we have not determined $P(q)$ in the presence of a magnetic field within the MKA, we can conclude from the behavior of A that $P(q)$ must have in the MKA exactly the same features that we just described for the Monte Carlo simulations. Indeed, it is easy to show that A becomes large if most samples have a $P(q)$ with one narrow peak at q_0, and some samples have two peaks. For those samples with one peak, we have a small variance of q,

$$\chi_s \equiv \langle q^2 - q_0^2 \rangle,$$

which is essentially sample independent. For those samples with two peaks, we have a large variance χ_l which is different for each sample. If the fraction of samples with two peaks is p, we obtain

$$A = \frac{(1-p)\chi_s^2 + p[\chi_l^2]}{\{(1-p)\chi_s + p[\chi_l]\}^2} - 1 \simeq \frac{p[\chi_l^2]}{\chi_s^2 + 2p\chi_s[\chi_l] + p^2[\chi_l]^2},$$

where we have kept only the leading terms. As long as p is not much smaller than $[\chi_l]/\chi_s$, A is of the order $1/p$. Thus, if χ_s is small and p is small but not too small, A is large. The second condition is satisfied if the field is such that a small fraction of samples have a second peak in $P(q)$; the first condition is better satisfied for larger L or smaller T. This explains why we observe the maximum of A for those h values where the contribution of the field to the free energy is comparable to that of the couplings, and why the maximum of A is larger for larger systems and lower temperatures. Of course, for some even larger value of L, we expect $P(q)$ to start having fewer sample-to-sample fluctuations, because the samples should become self-averaging. Then the argument will break down, and A should remain small. However, this range of system sizes seems to be beyond the reach of our simulations.

In conclusion, we have shown that there exists a wide range of parameters over which the degree of non-self-averaging appears large for system sizes typically used in computer simulations. We expect our results to be valid beyond the MKA. As we have argued for systems without a field [3,7], the apparent non-self-averaging must be attributed to the influence of the zero-field critical point. This influence reaches surprisingly far and creates a line in the h-J plane along which non-self-averaging is particularly large, and which is somewhat reminiscent of the de Almeida–Thouless line. We are here in agreement with Huse and Fisher [29] who already argued almost 10 years ago that Monte Carlo simulation data for a spin glass in a magnetic field are strongly affected by the critical point.

VI. DISCUSSION

We have shown that for the three-spin model as well as for the spin glass in a magnetic field a large degree of non-self-averaging found in computer simulations does not represent unequivocal evidence for RSB, but can be caused by finite-size effects. It seems, however, that a study of the non-self-averaging parameter A using Monte Carlo simulations might be able to discriminate between RSB and the droplet picture for three- and four-dimensional spin glasses. As we have shown, A has a maximum at T_c in zero field, and decreases again with decreasing temperature in the MKA. If there was a low-temperature phase with RSB, the low-temperature value for A should probably be larger than the critical value, and A should therefore increase with decreasing temperature. Also, for temperatures below T_c, we found that A has its maximum not at zero field, but at some finite field value. The degree of non-self-averaging decreases deep in the supposed low-temperature phase. We expect a similar behavior from the Monte Carlo simulations. This would be a hint that non-self-averaging is strongest along the boundary between the field-dominated and coupling-dominated regimes, and not in the region where one would expect a low-temperature phase with RSB.

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[1] E. Marinari, G. Parisi, F. Ricci-Tersenghi, and J.J. Ruiz-Lorenzo in *Spin Glasses and Random Fields*, edited by A.P. Young (World Scientific, Singapore, 1997).
[2] E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. Ruiz-Lorenzo, and F. Zuliani, J. Stat. Phys. **98**, 973 (2000).
[3] M.A. Moore, H. Bokil, and B. Drossel, Phys. Rev. Lett. **81**, 4252 (1998).
[4] H. Bokil A.J. Bray, B. Drossel, and M.A. Moore, Phys. Rev. Lett. **82**, 5174 (1999).
[5] H. Bokil, A.J. Bray, B. Drossel, and M.A. Moore, Phys. Rev. Lett. **82**, 5177 (1999).
[6] Barbara Drossel, Hemant Bokil, M.A. Moore, and A.J. Bray, Eur. Phys. J. B **13**, 369 (2000).
[7] Hemant Bokil, Barbara Drossel, and M.A. Moore, Phys. Rev. B **62**, 946 (2000).
[8] J. Houdayer and O.C. Martin, Europhys. Lett. **49**, 794 (2000).
[9] J.P. Bouchaud, e-print cond-mat/9910387.
[10] F. Krzakala and O.C. Martin, Phys. Rev. Lett. **85**, 3013 (2000).
[11] M. Palassini and A.P. Young, Phys. Rev. Lett. **85**, 3017 (2000).
[12] H.G. Katzgraber, M. Palassini, and A.P. Young, e-print cond-mat/000713.
[13] E. Marinari, G. Parisi, and F. Zuliani, J. Phys. A **31**, 1881 (1998).

[14] E. Marinari, C. Naitza, and F. Zuliani, J. Phys. A **31**, 6355 (1998).
[15] M. Marinari, C. Naitza, F. Zuliani, G. Parisi, M. Picco, and F. Ritort, Phys. Rev. Lett. **81**, 1698 (1998).
[16] G. Parisi, M. Picco, and F. Ritort, Phys. Rev. E **60**, 58 (1999).
[17] J.-P. Bouchaud, L. F. Cugliandolo, J. Kurchan, and M. Mezard, in *Spin Glasses and Random Fields* (Ref. [1]), p. 161.
[18] T.R. Kirkpatrick and P.G. Wolynes, Phys. Rev. B **36**, 8552 (1987).
[19] T.R. Kirkpatrick and D. Thirumalai, Phys. Rev. B **36**, 5388 (1987); T.R. Kirkpatrick and P. Wolynes, Phys. Rev. A **35**, 3072 (1987).
[20] W. Götze and L. Sjögren, Rep. Prog. Phys. **55**, 241 (1992).
[21] W. Kauzmann, Chem. Rev. **43**, 219 (1948).
[22] L. Santen and W. Krauth, Nature (London) **405**, 550 (2000).
[23] M. Marinari, C. Naitza, F. Zuliani, G. Parisi, M. Picco, and F. Ritort, Phys. Rev. Lett. **82**, 5175 (1999).
[24] B.W. Southern and A.P. Young, J. Phys. C **10**, 2179 (1977).
[25] J. Houdayer and O.C. Martin, Phys. Rev. Lett. **82**, 4934 (1999).
[26] E. Marinari, G. Parisi, and F. Zuliani, Phys. Rev. Lett. **84**, 1056 (2000).
[27] J. Houdayer and O.C. Martin, Phys. Rev. Lett. **84**, 1057 (2000).
[28] E. Marinari, G. Parisi, and J.J. Ruiz-Lorenzo, Phys. Rev. B **58**, 14 852 (1998).
[29] D.A. Huse and D.S. Fisher, J. Phys. I **1**, 621 (1991).