
Numerical simulations of spin glasses: methods and some recent results

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Summary. After a introduction to spin glasses, a discussion will be given of the Monte Carlo techniques used to study them. I will include discussions of parallel tempering, used to speed up equilibration, and finite size scaling, used to extrapolate from results on finite size systems to the thermodynamic limit. I will also describe some recent results on the absence of a transition in a magnetic field (Almeida-Thouless line).

1 Introduction

This talk will provide an introduction to spin glasses[1, 2], why they are interesting, and what are the computational challenges in studying them numerically. At the end I will describe one topic that I have recently been working on; whether or not there is a phase transition in a spin glass in a magnetic field, the so-called Almeida-Thouless (AT) line.

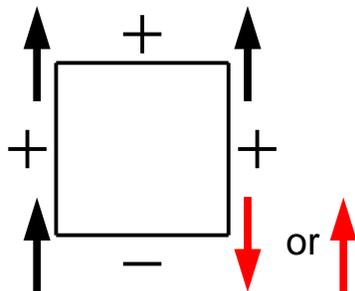


Fig. 1. A toy model which shows frustration. If the interaction on the bond is a “+”, the spins want to be parallel and if it is a “-” they want to be antiparallel. Clearly all these conditions can not be met so there is competition or “frustration”.

It is generally agreed that for a system to be a spin glass it needs two ingredients: randomness and “frustration”. Frustration refers to the competition between interactions which means that no configuration of the system will simultaneously minimize each term in the Hamiltonian. A toy example illustrating frustration is shown in Fig. 1. Here the arrows refer to Ising spins which can point up or down, $S_i = \pm 1$, and the interaction between them is ferromagnetic (preferring parallel spin alignment) if it is indicated by a “+” and antiferromagnetic (preferring antiparallel spin alignment) if indicated by a “-”. A spin glass therefore has a random mixture of ferro- and antiferromagnetic tendencies. In the figure, no configuration of the spins will minimize the energy of each bond because there is an odd number of negative bonds.

It is clear from this example that if one considers a large lattice, determining the exact ground state of a spin glass is highly non-trivial. In fact, it is an example of what computer scientists call a combinatorial optimization problem. There has been overlap of ideas between spin glasses and the theory of combinatorial optimization with computer scientists providing efficient code for determining spin glass ground states[3] (in certain cases) and spin glass physics providing the inspiration for efficient algorithms[4] for some optimization problems.

Just as the determination of the true ground state is very hard, it is clear that there are many states fairly close by in energy to it and which, it turns out, can differ in the orientation of a large number of spins. As a result an important concept in spin glasses is that of the “energy landscape”, which is a projection on to a single axis of the variation of the energy (strictly speaking at finite temperature a suitably defined free energy). This has a complicated structure with minima (valleys) separated by barriers, see Fig. 2.

Experimentally, there are different types of materials with the ingredients of randomness and frustration needed to form a spin glass. For example:

- Metals:
Diluted magnetic atoms, e.g. Mn, in a non-magnetic metal such as Cu, interact with the RKKY interaction whose sign depends on the distance between the atoms.
- Insulators:
An example is $\text{Fe}_{0.5}\text{Mn}_{0.5}\text{TiO}_3$, which comprises hexagonal layers. The spins align perpendicular to layers (hence it is *Ising*-like). Since it is an insulator, the interactions are short-range. Within a layer, spins in pure $\text{Fe}_{0.5}\text{TiO}_3$ are ferromagnetically coupled whereas spins in pure $\text{Mn}_{0.5}\text{TiO}_3$ are antiferromagnetically coupled. Hence a random mixture of Fe and Mn gives a spin glass.

We should mention, at this point, that two types of averaging have to be done in random systems. First of all we need to perform the usual statistical mechanics average for a given set of random interactions. Precise values of measured quantities will depend on the particular set of random interactions, though many quantities, such as the free energy or energy, will be

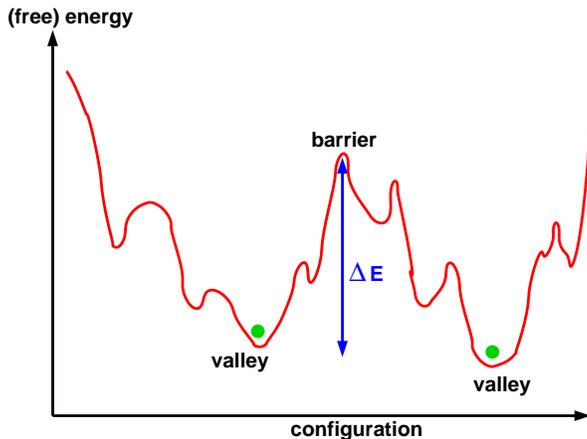


Fig. 2. A cartoon of the “energy landscape” in a spin glass. As the spin configuration is changed, represented by moving along the horizontal axis, the system goes through local minima (which have very similar energy but differ in the orientation of a large number of spins) separated by barriers. At low temperature the system easily gets trapped in one of the minima leading to slow dynamics.

“self-averaging”, i.e. the sample to sample fluctuation will be small compared with the average value (generally down by of order $1/\sqrt{N}$ where N is the number of spins). However, even for self averaging quantities, the sample to sample fluctuations will not be negligible for the small lattice sizes that can be simulated, and so we need to perform an average over the disorder, by repeating the simulation many times with different choices for the interactions. We denote the thermal average by $\langle \dots \rangle$ and the disorder average by $[\dots]_{\text{av}}$.

Next we discuss the main experimental features of spin glasses. At low temperatures, the dynamics of spin glasses becomes very slow, so the system is not in equilibrium. This non-equilibrium behavior has been extensively studied in recent years. Of particular note has been the study of “aging” in spin glasses, pioneered by the Uppsala group [5]. One cools the system to low temperature and waits for a “waiting time” t_w . The system is then perturbed in some way, e.g. by applying a magnetic field, and the subsequent response is measured. It is found that the nature of the response depends on t_w , providing clear evidence that the system was not in equilibrium. However, in this talk, I will not be discussing this interesting non-equilibrium behavior.

If one measures the ac susceptibility $\chi(\omega)$ one finds a Curie, or Curie-Weiss behavior at high temperature followed by a fairly sharp cusp at a freezing temperature $T_f(\omega)$ which depends weakly on the frequency ω . There has been extensive discussion as to whether this represents “gradual freezing”, i.e. the slowing down of the dynamics discussed above (of local entities), or whether the cusp indicates a sharp thermodynamic phase transition.

After considerable work, it became clear that a spin glass has a sharp phase transition at temperature $T = T_{SG}$, such that for $T < T_{SG}$ the spins freeze in some random-looking orientation. The spin glass order parameter can be taken to be

$$Q = [\langle S_i \rangle^2]_{\text{av}}. \quad (1)$$

To evaluate the square of the thermal average in simulations without bias, two copies of the system, “1” and “2”, with the same bonds are studied, and $Q = [\langle q \rangle]_{\text{av}}$, where the microscopic order parameter (spin overlap) is given by

$$q = \frac{1}{N} \sum_i S_i^{(1)} S_i^{(2)}. \quad (2)$$

The transition temperature T_{SG} is equal to the zero frequency limit of the freezing temperature $T_f(\omega)$. As $T \rightarrow T_{SG}^+$, the spin glass correlation length, the distance over which spins are correlated, diverges. We should mention, though, that some pairs of spins will be ferromagnetically correlated, whereas others, the same distance apart, will be antiferromagnetically correlated because they have different environments. A related quantity which diverges, therefore, is the *spin glass susceptibility*

$$\chi_{\text{SG}} = \frac{1}{N} \sum_{\langle i,j \rangle} [\langle S_i S_j \rangle^2]_{\text{av}}, \quad (3)$$

(notice the square) which is accessible in simulations. It is also essentially the same as the *non-linear susceptibility*, χ_{nl} , which can be measured experimentally and is defined by the coefficient of h^3 in the expansion of the magnetization m ,

$$m = \chi h - \chi_{nl} h^3 + \dots, \quad (4)$$

where h is the magnetic field. We expect that χ_{nl} and χ_{SG} diverge at T_{SG} like

$$\chi_{nl} \sim (T - T_{SG})^{-\gamma}, \quad (5)$$

where γ is a critical exponent. This divergent behavior has been seen in many experiments. A nice example is the data of Omari et al. [6] on 1% Mn in Cu which shows a clear divergence.

2 Model and Theory

Most theoretical work has used the simplest model with the properties of randomness and frustration, which is due to Edwards and Anderson [7]:

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j, \quad (6)$$

in which the spins S_i lie on the sites of a regular lattice with $N = L^d$ sites with periodic boundary conditions. The interactions J_{ij} , which we assume here to be between nearest neighbors only, are independent random variables with mean and standard deviation given by

$$[J_{ij}]_{\text{av}} = 0; \quad [J_{ij}^2]_{\text{av}}^{1/2} = J (= 1). \quad (7)$$

A zero mean is chosen to avoid any bias towards ferromagnetism or anti-ferromagnetism, and it is convenient, in the simulations, to take a Gaussian distribution for the J_{ij} , though sometimes a bimodal distribution, $J_{ij} = \pm 1$ with equal probability, is also used. Here we take Ising spins, $S_i = \pm 1$, though classical m -component vector spins are also of interest, see e.g. Ref. [8].

The infinite range version of the Edwards Anderson model, proposed by Sherrington and Kirkpatrick[9] (SK), has also been extensively studied. SK argued that the exact solution of this model could be considered the mean field theory for spin glasses, and that the actual behavior of a short range system may not be very different. These assumptions are true for ferromagnets. In fact, the exact solution of the SK model, found by Parisi[10, 11] is very complicated. To average over the disorder analytically, the “replica trick” is used, and the Parisi solution involves “replica symmetry breaking” (RSB) which seems to physically correspond to the phase space being divided up into different regions with infinite barriers in between. Hence, in a finite time, the system will stay confined within a single region (“ergodic component”).

One of the surprising features of the SK model is that there is a transition in a magnetic field the Almeida Thouless (AT)[12] line, separating a complicated region with RSB (and hence a spectrum of relaxation times extending to infinity) below the line and a simpler region without RSB (and only finite relaxation times) above the line. Note that there is no symmetry change here since the order parameter q is non-zero on both sides of the line. The AT line therefore represents a pure ergodic–non ergodic transition without any symmetry change.

A lot of discussion has arisen as to the nature of the spin glass state below T_{SG} in short range spin glasses. Two main scenarios have been proposed.

- According to the RSB scenario, the behavior of short range spin glasses is very similar to that of the SK model. In particular there is an AT line in a magnetic field.
- In the “droplet picture”[13, 14], attention is focused on the geometrical aspects of the low energy excitations, which do not exist in an infinite range model. A number of properties are expected to be different in the droplet picture compared with the RSB picture; in particular a magnetic field rounds out the spin glass transition so there is no AT line.

A third, intermediate scenario, called the “TNT” (Trivial-Non Trivial)[15, 16], has also been proposed. It is difficult to clearly determine numerically which scenario is correct because they refer to the equilibrium state, which

is never achieved for large systems. Hence the system sizes are quite modest, and there is an uncertainty whether they are big enough for the asymptotic (i.e. $L \rightarrow \infty$) limit to have been reached.

3 Numerical Aspects

3.1 Speeding up the dynamics

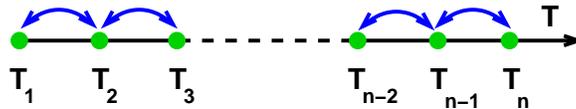


Fig. 3. Temperature swaps in the parallel tempering approach.

We have mentioned that spin glass dynamics is slow at low temperatures on account of the complicated energy landscape. To speed things up most spin glass simulations now use the “parallel tempering” [17, 18] method in which one simulates n copies of the system, with the same bonds, at different temperatures, see Fig. 3. In addition to the usual single spin flip Monte Carlo moves for each copy, one also performs global moves in which configurations at neighboring temperatures are swapped, with a probability which satisfies the detailed balance condition for the ensemble of copies. The detailed balance condition ensures that the ensemble eventually comes to thermal equilibrium. However, if one looks at a single set of spins its temperature is not constant but performs a random walk between the minimum and maximum temperatures, $T_{min} \equiv T_1$ and $T_{max} \equiv T_n$ respectively. T_{max} is chosen to be sufficiently high that the system equilibrates fast, and so, if we follow a given set of spins from T_{min} up to T_{max} and back down again to T_{min} , there is no reason for it to be in the same valley when it returns to T_{min} as was at the beginning, because the configuration was completely randomized at T_{max} .

In practice, parallel tempering enables us to simulate intermediate size systems, e.g. $\sim 10^3$ spins, at low temperatures. Unfortunately, it still does not enable us to study very large system sizes.

3.2 Test for Equilibration

Even with parallel tempering, Monte Carlo dynamics is quite slow at low temperatures, and it is desirable to have a sound criterion for deciding whether the system has equilibrated. The usual approach is to increase the length of the simulation until the results don’t seem to change. However, this can

potentially be unreliable if measured quantities change only very slowly with number of Monte Carlo sweeps; e.g. results from runs of t and $2t$ sweeps could give the same results within error bars but could still be far from equilibrium.

For a spin glass with a Gaussian distribution of bonds an alternative approach has been developed[19]. The average energy U involves terms like $-[J_{ij}\langle S_i S_j \rangle]_{\text{av}}$. The disorder average is with respect to the weight $\int dJ_{ij} \exp(-J_{ij}^2/2)$ and so one can integrate the energy by parts with respect to the J_{ij} . This gives

$$U = U(q_l) \equiv -\frac{z}{2} \frac{1 - q_l}{T}, \quad (8)$$

where q_l is the ‘‘link overlap’’

$$q_l = \frac{1}{N_b} \sum_{\langle i,j \rangle} [\langle S_i S_j \rangle^2]_{\text{av}}, \quad (9)$$

the sum is over nearest neighbor pairs, and $N_b = Nz/2$ is the number of such pairs. Here z is the number of neighbors per site, e.g. 6 for the simple cubic lattice.

Clearly U will approach its equilibrium value from above. To evaluate the average of the square in Eq. (9) two separate copies (‘‘1’’ and ‘‘2’’) are simulated and $\langle S_i S_j \rangle^2$ is evaluated as $\langle S_i^{(1)} S_j^{(1)} S_i^{(2)} S_j^{(2)} \rangle$. Starting the spins in the two copies in random directions, it is plausible that q_l approaches its equilibrium value from below. Hence we expect the two sides in Eq. (8) to approach their common equilibrium value from opposite sides, and, once they agree, not to change further. This seems to be correct as shown in Fig. 4.

3.3 Finite size scaling

In order to locate and analyze a critical point, we use the technique of finite size scaling to extrapolate results from a range of finite sizes to the thermodynamic limit. A particularly useful quantity turns out to be the correlation length of the finite size system ξ_L . One can extract this by Fourier transforming the spin glass correlation function

$$\chi_{\text{SG}}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} [\langle S_i S_j \rangle^2]_{\text{av}} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \quad (10)$$

Above T_{SG} and a long wavelengths we expect this to have an Ornstein-Zernicke form

$$\chi_{\text{SG}}(\mathbf{k}) \propto (\xi_L^{-2} + k^2) \quad (11)$$

and so we *define* ξ_L for all T to be

$$\xi_L^2 = \frac{1}{2(1 - \cos(k_{\min}))} \left(\frac{\chi_{\text{SG}}(0)}{\chi_{\text{SG}}(\mathbf{k}_{\min})} - 1 \right) \quad (12)$$

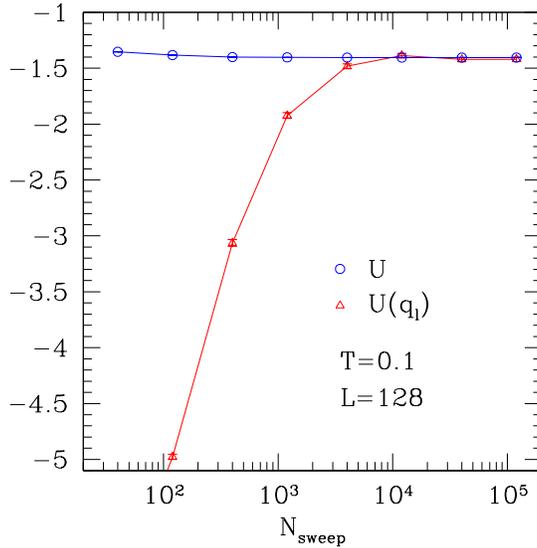


Fig. 4. Equilibration test in a spin glass with Gaussian interactions. This is actually for a one-dimensional model with long-range, power law interactions. (Adapted from [20]).

where $\mathbf{k}_{\min} = \frac{2\pi}{L}(1, 0, 0)$ is the smallest non-zero wavevector. A factor of k_{\min}^2 has been replaced by $2(1 - \cos(k_{\min}))$ since this incorporates the periodicity of $\chi_{\text{SG}}(\mathbf{k})$ in the repeated Brillouin zone.

The results for the correlation lengths will be analyzed according to finite-size scaling (FSS). The basic assumption of FSS is that the size dependence comes from the ratio L/ξ_{bulk} where

$$\xi_{\text{bulk}} \sim (T - T_{\text{SG}})^{-\nu} \quad (13)$$

is the *bulk* correlation length. In particular, the *finite-size* correlation length is expected to vary as

$$\frac{\xi_L}{L} = X \left(L^{1/\nu} (T - T_{\text{SG}}) \right), \quad (14)$$

since ξ_L/L is dimensionless (and so has no power of L multiplying the scaling function X). In particular, it is reasonable to expect that $\xi_L \propto L$ at the critical point, since L is the only length scale left in the problem (ξ_{bulk} is infinite and the lattice spacing is assumed to be unimportant when ξ_L is large).

From Eq. (14), data for ξ_L/L for different sizes should intersect at T_{SG} and splay out below T_{SG} .

3.4 Evidence for a finite transition temperature

Calculating the correlation length is an excellent technique to locate the critical point. As discussed in the previous subsection, the data should intersect at T_{SG} and splay out again at lower temperatures. This indeed occurs in the three dimensional Ising spin glass as shown in Fig. 5.

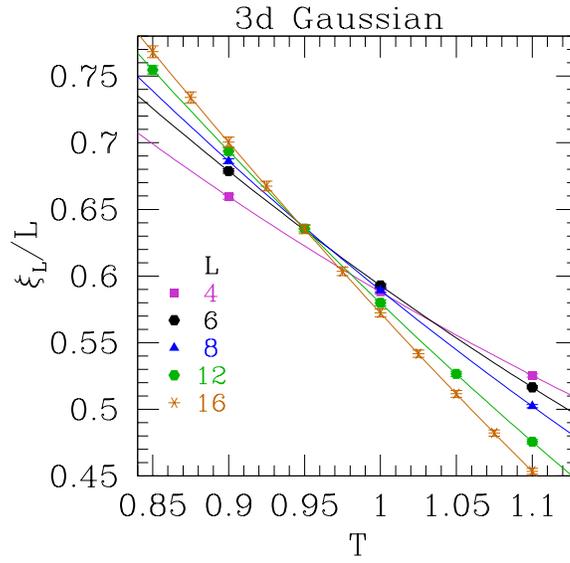


Fig. 5. Finite size scaling of the correlation length used to locate the critical point in the three-dimensional Ising spin glass with Gaussian interactions. (From Katzgraber and Young (unpublished)).

Use of the correlation length to locate the transition temperature in spin glasses was pioneered by Ballesteros et al.[21] for the $\pm J$ distribution. Prior to the work of Ballesteros et al., determination of T_{SG} generally used the “Binder ratio”, a dimensionless ratio of the moments of the order parameter distribution which has a finite size scaling of the same form as in Eq. (14). However, this gives much less convincing demonstration of a transition, see Fig. 6 which shows data from Marinari et al. [22] for the Gaussian distribution.

4 Absence of a phase transition in a magnetic field

In the last part of this lecture, I will describe some recent work with Helmut Katzgraber[23] on the possible existence of a transition in a magnetic field

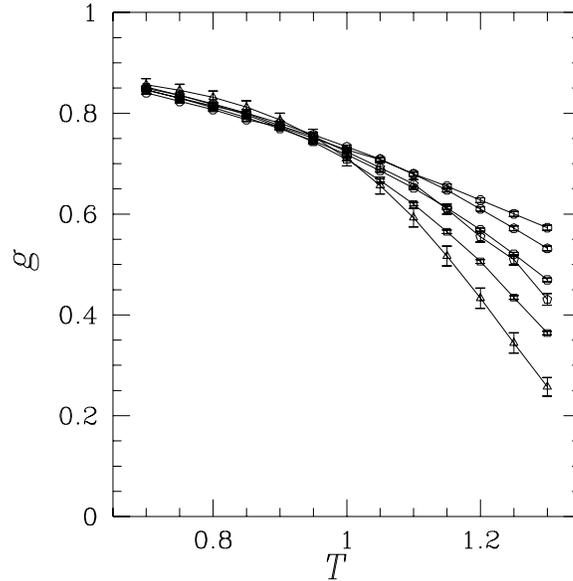


Fig. 6. Data for the Binder ratio length of the Ising spin glass with Gaussian interactions, from Marinari et al.[22]. The data merge but do not clearly splay out on the low- T side, unlike the results for the correlation length shown in Fig. 5.

(AT line) in a three-dimensional Ising spin glass. You will recall from the first part of the talk that an AT line is predicted by the RSB scenario for the spin glass state but not by the droplet scenario, see Fig. 7.

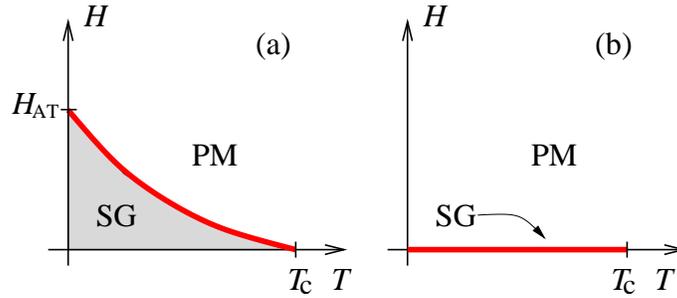


Fig. 7. Part (a) shows the phase diagram of a spin glass in a magnetic field expected in the RSB scenario. The line of phase transitions is called the AT line. Part (b) shows the analogous phase diagram in the droplet picture. There is no AT line.

The Hamiltonian is now

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i h_i S_i, \tag{15}$$

where h_i is the magnetic field on site i . Usually treatments of the AT line consider a uniform field, but we take a Gaussian distribution with zero mean and standard deviation H_r because, in this case, a generalization[23] of the equilibration test discussed above can be applied. For a symmetric distribution of bonds (used here), the *sign* of h_i can be “gauged away” so a uniform field is completely equivalent to a bimodal distribution of fields with $h_i = \pm H$. Our choice of a Gaussian distribution, which still has an AT line in mean-field theory, also puts disorder into the *magnitude* of the h_i .

In a magnetic field, where $\langle S_i \rangle$ is non-zero, the appropriate expression for $\chi_{\text{SG}}(\mathbf{k})$ is

$$\chi_{\text{SG}}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} \left[\left(\langle S_i S_j \rangle_T - \langle S_i \rangle_T \langle S_j \rangle_T \right)^2 \right]_{\text{av}} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}, \quad (16)$$

In order to evaluate the products of thermal averages without bias, 4 copies with the same bonds (at each temperature) are simulated. The expression for ξ_L is then the same, Eq. (12), as before.

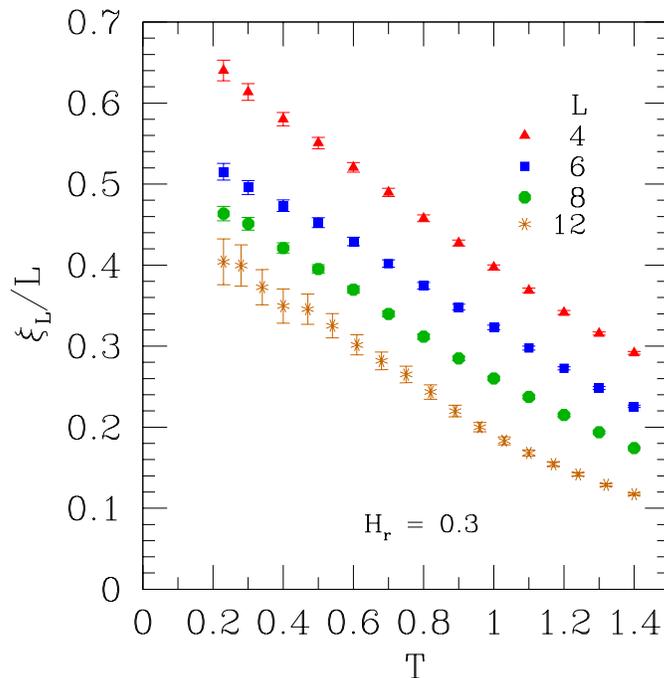


Fig. 8. Data for ξ_L/L for $H_r = 0.3$ for different sizes. Note that in contrast to the zero-field data shown earlier there is no sign of intersections down to the lowest temperature $T = 0.23$. (From Ref.[23].)

Data for $H_r = 0.3$ are shown in Fig. 8. In contrast to the zero field results presented earlier in the talk, there is no sign of an intersection down to very low temperatures. Similar results have been found for even smaller values of the field. This strongly suggests that there is no AT line in three-dimensional spin glasses.

This result is compatible with the droplet picture. However, other numerical results do not seem to be consistent with it. In particular the order parameter in the Parisi RSB theory is actually a probability distribution $P(q)$ with a delta function at $q = q_{EA}$ corresponding to ordering in a single valley, and a continuous part, with a non-zero weight at $q = 0$, coming when one of the two copies used to determine q according to Eq. (2) is in one valley and the other copy is in another valley. In the droplet picture, the weight at $q = 0$ vanishes with system size like $L^{-\theta}$ where θ is a positive exponent. Simulation results for $P(q)$, see e.g. Refs. [19, 20], agree much better with the RSB picture.

Hence the situation are rather confusing, and agree best with the intermediate ‘‘TNT’’ picture[15, 16]. However, it is also possible that the system sizes that can be studied have not reached ‘‘asymptopia’’, where the behavior of the $L \rightarrow \infty$ limit becomes apparent. Unfortunately, there seem to be no ideas at present for algorithms which are so superior than the present ones that *significantly* bigger sizes can be studied, though *incremental* improvement can be expected.

5 Conclusions

The spin glass problem is hard. Analytical results are few and far between, and numerical studies are usually limited to quite small sizes. In fact, finding the ground state of a spin glass in three or more dimensions belongs to a hard class of optimization problems (NP-complete), for which it is believed that there is no algorithm which can find the exact ground state in a time which increases with only a power of the system size. However, the two-dimensional Ising glass is not NP-complete and there are efficient polynomial-time algorithms for determining the ground state[3]. As a result, lattices with of order a million spins can be studied in two dimensions, whereas in three dimensions the largest sizes have a few thousand spins.

In finite temperature Monte Carlo simulations, parallel tempering helps, but does not fully overcome the problem of slow dynamics. The results of simulations on modest-sized lattices below T_{SG} are not fully consistent with either the RSB or the droplet scenarios.

Acknowledgments

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