Spin Glasses: A Computational Challenge for the 21st Century

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Abstract

I discuss the computational challenges of the spin glass problem, and illustrate them with two examples from my recent work.

I. INTRODUCTION

In this talk I will discuss the computational challenges of the spin glass problem, which have occupied us for the last quarter of the 20th century and look set to continue to occupy us well into the 21st. I will illustrate these challenges by briefly discussing two examples from my own recent work.

Spin glasses [1] are systems with both randomness and "frustration", or competition, between the spins. These ingredients are found to give rise to the following behavior:

- A complicated energy landscape with "valleys" separated by barriers which are only traversed rarely at low temperatures. There are configurations with an energy close to that of the ground state, but which differ from the ground state in the orientation of a large number of spins.

- Because of the complicated energy landscape the dynamics is very slow, and the system is never fully in equilibrium at low temperature.

- There is a phase transition with a divergence in a non-linear response function. Although spin glasses bear some resemblance to "window glasses", including the name, it appears that window glasses do not have thermodynamic transition, at least in the temperature region where experiments are near equilibrium. Rather, for window glasses, the observations show a rapidly increasing relaxation time without a diverging correlation length. Hence the analogy between window glasses and spin glasses should not be pushed too far.

Work on spin glasses has focussed on several issues, the most important of which seem to be:

1. **Is there a phase transition?** The existence of a finite temperature phase transition with a divergence of the non-linear susceptibility has been shown for a three-dimensional Ising spin glass, with the most convincing data being that of Ballesteros et al. [2]. It is very easy so show from simulations that a transition occurs in higher dimensions. In two-dimensions, however, which I will discuss in the next section, the transition occurs only at $T = 0$, with the spin glass correlation length diverging in this limit.

2. **How can one characterize the low-T spin glass phase?** A lot of discussion has taken place regarding the nature of the low temperature spin glass phase below T_c. Two principal theories have been discussed, the "droplet theory" of Fisher and Huse [3] and others [4], and the "replica symmetry breaking theory" (RSB) of Parisi [5,6]. While spin glasses are characterized by the existence of large-scale excitations which cost only a small energy, these two approaches differ in the way the typical energy varies with the length scale of the excitation, and in the fractal dimension of the surface of the excitations. Space limitations prevent a discussion of this important topic here, and I simply refer the reader to some recent literature [7–12].

3. **What is the nature of the non-equilibrium dynamics?** At low temperatures, and certainly below the transition temperature T_c, spin glasses are never fully in e-quilibrium. It is therefore important to study *non-equilibrium* effects in a controlled

manner. Particularly useful have been the "aging" experiments pioneered by Norblad et al. [13], in which one studies, in a cooling experiment, how properties depend on the time that the system waited at a certain temperature. One of the remarkable aspects, still not understood, is the "memory" effect [14]. To explain this, suppose one measures the ac susceptibility, $\chi_{\rm ac}$, while slowly cooling the system, and waits for an additional time at some temperature T_w, below T_c. During the waiting period the value of $\chi_{\rm ac}$ decreases. On further cooling $\chi_{\rm ac}$ increases to the value it would have had without the wait at T_w, which is called "rejuvenation". On rewarming, $\chi_{\rm ac}$ tracks the values it had on cooling, *including the dip at* T_w. This indicates that that, while at lower temperature, the system maintained a memory that it waited at T_w. Surprisingly this behavior has *not* been reproduced by numerical simulations [15]. This may be because the simulations run for much shorter times, relative to the microscopic time, than the experiments, but a resolution of this difference is one of the most important problems in spin glasses.

It is believed that the important ingredients in a spin glass are randomness and frustration. Most theoretical work has therefore used the simplest model with these ingredients, due to Edwards and Anderson [16]. For the case of Ising spins, where $S_i = \pm 1$, this is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \, , \tag{1}$$

where the spins S_i lie on the sites of a lattice with $N = L^d$ sites in d dimensions with periodic boundary conditions. The interactions J_{ij} are, for simplicity, taken between nearest neighbor sites only, and are assumed to be independent random variables. To avoid ferromagnetism or anti-ferromagnetism we set the mean equal to zero, and take the variance to be unity which sets the temperature scale, i.e.

$$[J_{ij}]_{\rm av} = 0, \qquad [J_{ij}^2]_{\rm av} = 1 \, , \tag{2}$$

where $[\cdots]_{\rm av}$ denotes an average over the disorder. Common choices for the distribution of disorder are a Gaussian, and the $\pm J$ distribution, where $J_{ij} = \pm 1$ with equal probability.

The ground state of the $\pm J$ model has a high degeneracy giving rise to a finite entropy per spin at $T = 0$.

In the next two sections, I will illustrate the computational challenges of the spin glass problem with a discussion of two pieces of my recent work:

1. The nature of the zero temperature transition in the two-dimensional Ising spin glass, and the difference brought about if the model has a macroscopic ground state degeneracy [17].

2. The effects of a macroscopic ground state degeneracy on the behavior of the spin glass in three dimensions at low temperature, well below T_c [18].

II. DEFECT ENERGIES IN TWO-DIMENSIONS

The spin glass problem at $T = 0$, i.e. the problem of finding the ground state, is non-trivial because of frustration. It is an example of what computer scientists call an "optimization problem". Certain optimization problems are found to be in a class denoted by "P", for which there is an algorithm that determines the ground state in a time proportional to a power of the size of the system. For problems in another class, called "NP-hard", no polynomial algorithms have been found, and they probably do not exist though this has not yet been proved rigorously. To prove this (or the converse) is one of the grand challenges of computer science. Any problem in the NP-hard class can be transformed into any other in polynomial time, so a polynomial time algorithm for one of them would solve all of them all of them in polynomial time. The computer time for an NP-hard problem presumably varies exponentially with the system size, and so, in general, one can only study much smaller systems than is possible for problems with a polynomial algorithm.

In two dimensions, and with boundary conditions which do not wrap round in both directions (the bonds must be drawable as a "planar graph"), there are efficient polynomial-time "matching" algorithms [19,20] for finding the ground state. For a review see Ref. [21].

To our knowledge the "world record" for a spin glass ground state is [22] size 1800×1800. In my work with Hartmann [17], we used the LEDA [23] libraries, which require quite a lot of memory, so we were limited to size 480×480. As we shall see in the next section, this is still very large compared with the sizes that can be tackled in three dimensions, which is in the NP-hard class.

We are not interested in the ground state *per se* but rather in the large scale, low energy excitations out of the ground state. These can be induced by a change in the boundary conditions, followed by a recomputation of the ground state. To be precise, a "defect energy" [24–26] is calculated in the following way. For each sample, we determine

$$\delta E = E_P - E_{AP}, \tag{3}$$

where E_P is the (total) energy with periodic boundary conditions and E_{AP} is the energy with anti-periodic boundary conditions. Since δE can have either sign for spin glass, we take the absolute value before averaging over disorder to obtain the defect energy

$$\Delta E = [\,|\delta E|\,]_{av}. \tag{4}$$

One expects that

$$\Delta E \sim L^{\theta}, \tag{5}$$

where θ is an exponent. If $\theta > 0$ then the spin glass state is quite rigid and should persist up to a finite temperature. However, if $\theta < 0$, large scale excitations cost almost no energy, so spin glass order will presumably break up at any finite-T, and hence $T_c = 0$.

Up to now, defect energy calculations have been carried out up to sizes $L = 32$ [27,28]. It seems useful to use the matching algorithm to study defect energies up to much larger sizes [17]. The boundary conditions in one direction have to be free, but in the other direction they are changed from periodic to anti-periodic. An example of a domain wall induced in this way for a $L = 320$ sample is shown in Fig. 1. The spins are flipped on one side of the domain wall when the boundary conditions are changed and not on the other.

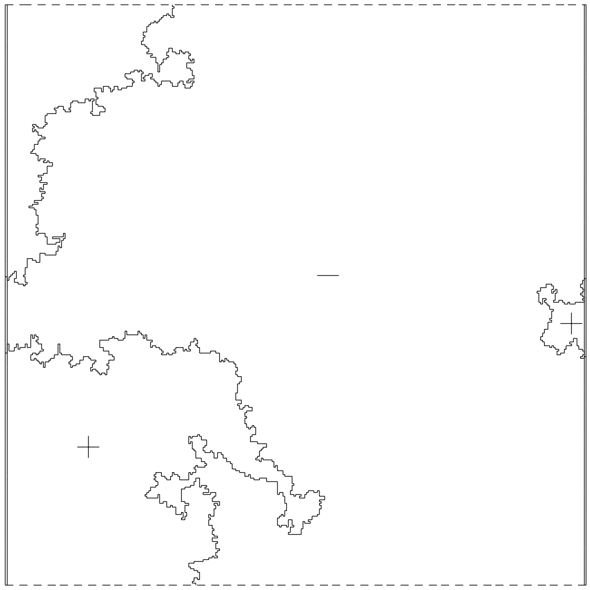

FIG. 1. A domain wall created in an $L = 320$ system with Gaussian interactions. Free boundary conditions are applied across the top and bottom edges (dashed lines) and periodic boundary conditions applied across the vertical edges (solid lines). The domain wall is induced by changing the periodic boundary conditions to antiperiodic, which is equivalent to changing the sign of the bonds which wrap round the system from left to right. The wall is really contiguous; since bonds wrap round the system from left to right, the left and right hand edges are really adjacent to each other.

We [17] find that, for a Gaussian distribution, $\theta = -0.282 \pm 0.002$, (where the error is only statistical), in agreement with earlier work. The negative value means that $T_c = 0$. However, for a $\pm J$ distribution, where the ground state has a high degeneracy and a finite ground state entropy per spin, we find $\theta = 0$. This means that $d = 2$ is the "lower critical dimension" (LCD), the borderline dimension above which there is a finite T_c and below which $T_c = 0$. Previous work [28] had clearly indicated that the $\pm J$ and Gaussian models behaved differently but did not get convincing evidence for $\theta = 0$. There are different scenarios for finite-T behavior at the LCD. One of these is an exponential divergence of the correlation length as $T \to 0$, which has been found by Saul and Kardar [30], and by Houdayer who used a sophisticated cluster Monte Carlo algorithm to study large systems, up to 100×100 down to very low temperature.

III. THE $\pm J$ MODEL IN THREE-DIMENSIONS

The determination of a spin glass ground state state in three dimensions is NP-hard. Heuristic algorithms, which have some features in common with evolution and so are called "genetic" algorithms, seem to be the most promising, and with them one can study system sizes up to about 12^3, a much smaller number of spins than in two dimensions. One finds [25,26,31,32] that $\theta > 0$, indicating a finite-T_c, which has also been verified directly by Monte Carlo simulations [2]. Since numerical results on such small lattices are susceptible to corrections to finite size scaling, the numerical data has not, however, given a generally accepted picture of the spin glass state *below* T_c.

In the rest of this section I will discuss how one can get information about *finite temperature* properties from Monte Carlo simulations. The difficulty is that the system becomes trapped, at low temperature, in one of the valleys in configuration space. In order to sample different valleys more quickly it is necessary that the energy (per spin) fluctuates by more than the small ($\sim 1/\sqrt{N}$) amount permitted by the canonical distribution. The most popular approach goes under the name of "parallel tempering" (also called "replica Monte Carlo") [33,34]. In this technique, one simulates several identical replicas of the system at different temperatures, and, in addition to the usual local moves, one performs global moves in which the temperatures of two replicas (with adjacent temperatures) are exchanged. It turns out to be straightforward to design an algorithm which satisfies the detailed balance condition, and it will also have a good acceptance ratio if the temperatures are fairly close together. In this way, the temperature (and hence energy) of a given replica wanders up and down in a random manner, and each time the temperature goes low the system is likely to end up in a different valley of the energy landscape. Thus different valleys are sampled in much less time than it would take for the system to fluctuate between valleys if the temperature stayed fixed.

A useful quantity to calculate, is the distribution of the spin glass order parameter, q, where

$$q = \frac{1}{N}\sum_{i=1}^{N} S_i^{(1)} S_i^{(2)}, \tag{6}$$

where “1” and “2” denote two copies of the system with the same interactions and the same temperature. In the thermodynamic limit, the order parameter distribution $P(q)$ is predicted to be single delta function at $q = q_{EA}$ in the droplet picture, whereas the RSB picture predicts, in addition, a continuous part (“tail”) extending down to $q = 0$. The delta function comes from overlap between spin configurations in a single “pure state”, while the continuous part is due to overlap between spin configurations in different pure states. In RSB several pure states have a significant statistical weight, while only one contributes in the droplet picture for large L. In the droplet picture, the weight in the tail is expected to vanish for $L \to \infty$ like $L^{-\theta}$ where $\theta\,(> 0)$ is the exponent introduced in the previous section.

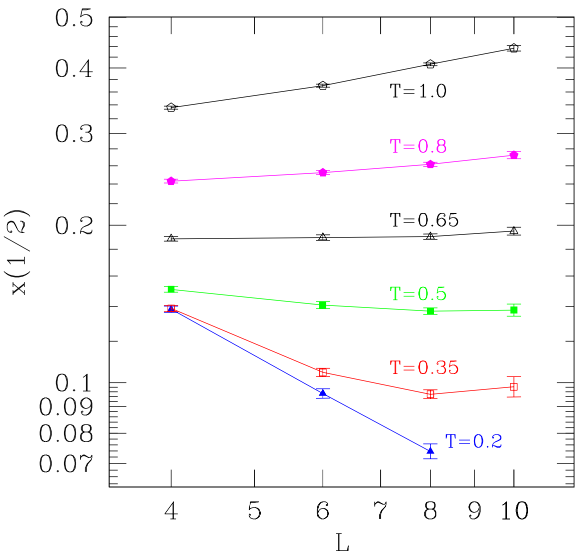

FIG. 2. Log-log plot of $x(1/2)$, the average of $P(q)$ over $|q| \le 1/2$, against L for the 3-d Ising spin glass with a $\pm J$ distribution. From Ref. [18].

Simulations at low-T [35] using parallel tempering for the Gaussian distribution found a non-trivial distribution with a weight in the tail, which did not decrease with increasing system size, as expected in RSB. However, it remains controversial whether this result persists for larger systems.

Palassini and I [18] looked at whether the macroscopic ground state degeneracy of the $\pm J$ model affects the nature of the spin glass state at low temperatures. Using parallel tempering we computed $P(0)$, the weight in the tail of $P(q)$ at small q, averaging over a range of q to improve statistics, and the results are shown in Fig. 2. We see a rapid decrease at low-T which then flattens off at larger sizes.

Krzakala and Martin [36] (KM) have argued that entropy effects cause one "valley" in the $T = 0$ energy landscape of the $\pm J$ model to dominate and consequently the weight in the tail to vanish at $T = 0$ like $L^{-\lambda}$, where λ is a positive exponent, even if the energy landscape is non-trivial. At finite-T, KM assume, based on the numerical results available, that the weight is finite for large L, so, by implication, there must be a crossover at some scale $L_c(T)$ from the $L^{-\lambda}$ behavior for $L < L_c(T)$ to a value independent of L at larger sizes. Our data is found to be consistent with this [18] with a value for λ of $\lambda = 0.9 \pm 0.1$. Hence for large enough sizes the ground state degeneracy of the $\pm J$ model does not alter the behavior of $P(q)$ compared with the Gaussian model; at $T = 0$, $P(q)$ is trivial in both cases, and for $T > 0$ it is non-trivial. However, at intermediate sizes, there is crossover behavior for the $\pm J$ model, which is not present for the Gaussian model.

The results of Ref. [18] are consistent with the zero temperature data of Berg [37] but differ somewhat from those of Hartmann [38]. They differ substantially from the finite-T Monte Carlo simulations of Hatano and Gubernatis [39], which may have not been fully equilibrated [40].

Finally, I should emphasize that it is still unclear whether the non-trivial $P(q)$ found in the numerics for small sizes, will persist to the thermodynamic limit.

IV. CHALLENGES FOR THE FUTURE

It would be very desirable to achieve the following:

- **Ground States.** Find better algorithms for NP-hard problems so that defect energy (and other ground state) calculations can be performed on larger systems for the 3-d spin glass.

- **Finite-Temperature.** Find a better algorithm than parallel tempering, so one can perform Monte Carlo simulations for larger sizes at low temperature than is currently possible. In two dimensions, the "replica exchange" method of Swendsen and Wang [41] and the technique of Houdayer [29] able one to find *finite* clusters of spins to flip to go from one valley to another. Using these methods larger systems can be simulated at lower temperatures than using parallel tempering. In higher dimensions though, the clusters percolate, and these techniques just reduce to parallel tempering. Can one modify these techniques in some way, so that they will also be effective in three and higher dimensions?

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REFERENCES

[1] K. Binder and A.P. Young, Rev. Mod. Phys. **58**, 801 (1986); M. Mezard, G. Parisi, M.A. Virasoro, *Spin glass theory and beyond*, (World Scientific, Singapore 1987); K.H. Fisher and J.A. Hertz, *Spin Glasses*, (Cambridge University Press, Cambridge 1991); A.P. Young (ed.), *Spin glasses and random fields*, (World Scientific, Singapore 1998).

[2] H. G. Ballesteros, A. Cruz, L. A. Fernandez, V. Martin-Mayor, J. Pech, J. J. Ruiz-Lorenzo, A. Tarancon, P. Tellez, C. L. Ullod and C. Ungil, Phys. Rev. B **62**, 14237 (2000) (cond-mat/0006211).

[3] D. S. Fisher and D. A. Huse, J. Phys. A. **20** L997 (1987); D. A. Huse and D. S. Fisher, J. Phys. A. **20** L1005 (1987); D. S. Fisher and D. A. Huse, Phys. Rev. B **38** 386 (1988).

[4] A. J. Bray and M. A. Moore, in *Heidelberg Colloquium on Glassy Dynamics and Optimization*, L. Van Hemmen and I. Morgenstern eds. (Springer-Verlag, Heidelberg, 1986).

[5] G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979); J. Phys. A **13**, 1101, 1887, L115 (1980; Phys. Rev. Lett. **50**, 1946 (1983).

[6] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).

[7] C. M. Newman and D. L. Stein, Phys. Rev. B **46**, 973 (1992); Phys. Rev. Lett., **76** 515 (1996); Phys. Rev. E **57** 1356 (1998).

[8] E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. Ruiz-Lorenzo and F. Zuliani, J. Stat. Phys. **98**, 973 (2000).

[9] F. Krzakala and O. C. Martin, Phys. Rev. Lett. **85**, 3013 (2000), (cond-mat/0002055).

[10] M. Palassini and A. P. Young, Phys. Rev. Lett. **85**, 3017 (2000), (cond-mat/0002134).

[11] E. Marinari and G. Parisi, Phys. Rev. Lett. **86**, 3887 (2001), (cond-mat/0007493).

[12] A. A. Middleton, Phys. Rev. B **63**, 060202(R) (2001).

[13] P. Norblad and P. Svendlidh in "*Spin Glasses and Random Fields*", A. P. Young Editor, World Scientific (1998).

[14] K. Jonason, E. Vincent, J. Hammann, J.-P. Bouchaud and P. Norblad, Phys. Rev. Lett.**31**, 3243 (1998). For a recent discussion of memory and rejuvenation effects in spin glasses see J.-P. Bouchaud, V. Dupuis, J. Hammann and E. Vincent, cond-mat/0106539.

[15] M. Picco, F. Ricchi-Tersenghi and F. Ritort, cond-mat/0005541.

[16] S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

[17] A. Hartmann and A. P. Young, cond-mat/0107308.

[18] M. Palassini and A. P. Young, Phys. Rev. B, **63**, 140408(R) (2001) (cond-mat/0012161).

[19] I. Bieche, R. Maynard, R. Rammal, and J.P. Uhry, J. Phys. A **13**, 2553 (1980).

[20] F. Barahona, J. Phys. A **15**, 3241 (1982).

[21] A.K. Hartmann and H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, Berlin, to be published 2001.

[22] R.G. Palmer and J. Adler, Int. J. Mod. Phys. C **10**, 667 (1999).

[23] K. Mehlhorn and St. Näher, *The LEDA Platform of Combinatorial and Geometric Computing*, Cambridge University Press, Cambridge 1999; see also `http://www.mpi-sb.mpg.de/LEDA/leda.html`.

[24] J. R. Banavar and M. Cieplak, Phys. Rev. Lett. **48**, 832 (1982).

[25] W.L. McMillan, Phys. Rev. B **30**, 476 (1984).

[26] A.J. Bray and M.A. Moore, J. Phys. C **17**, L463 (1984); A.J. Bray and M.A. Moore in *Heidelberg Colloquium on Glassy Dynamics*, J.L. van Hemmen and I. Morgenstern (eds), (Springer-Verlag, Heidelberg 1987).

[27] H. Rieger, L. Santen, U. Blasum-U, M. Diehl, M. Jünger, and G. Rinaldi, J. Phys. A

29, 3939-50 (1996).

[28] N. Kawashima and H. Rieger, Europhys. Lett. **39**, 85 (1997).

[29] J. Houdayer, preprint cond-mat/0101116.

[30] L. Saul and M. Kardar, Phys. Rev. E **48**, R3221 (1993). This work uses a polynomial-time algorithm which works with periodic boundary conditions in both directions (and even for $T > 0$) but is less efficient than the matching algorithm used here.

[31] M. Palassini and A. P. Young, Phys. Rev. Lett. **83**, 5126 (1999), (cond-mat/9906323).

[32] A.K. Hartmann, Phys. Rev. E **59**, 84 (1999).

[33] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan **65**, 1604 (1996).

[34] E. Marinari, in *Advances in Computer Simulation*, edited by J. Kertész and Imre Kondor (Springer-Verlag, Berlin 1998), p. 50, (cond-mat/9612010).

[35] H. G. Katzgraber, M. Palassini and A. P. Young, Phys. Rev. B **63**, 184422 (2001), (cond-mat/0007113).

[36] F. Krzakala and O. C. Martin, Europhysics Letters**53**, 749-755 (2001), (cond-mat/0010010).

[37] B. A. Berg, U. E. Hansmann and T. Celik, Phys. Rev. B **50**, 16444 (1994).

[38] A. K. Hartmann, Euro. Phys. Jour. B **13** 539 (2000).

[39] N. Hatano and J. E. Gubernatis, cond-mat/0008115.

[40] E. Marinari, G. Parisi, F. Ricci-Tersenghi and F. Zuliani, cond-mat/0011039.

[41] R. H. Swendsen and J. -S. Wang, Phys. Rev. Lett. **57**, 2607 (1986).