Is the Sherrington–Kirkpatrick model relevant for real spin glasses?

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A P Young

Department of Physics, University of California, Santa Cruz, CA 95064, USA

E-mail: peter@physics.ucsc.edu

Abstract

I describe the results of numerical simulations which test whether the Sherrington–Kirkpatrick model, which was solved by Parisi, applies to short-range spin glasses. I conclude that it probably does for dimension d greater than 6, but there appear to be some differences in lower dimensions. In particular, there does not appear to be the line of transitions in a magnetic field (AT line) which is seen in the SK model.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

It was a pleasure to give this talk at the meeting honoring the scientific contributions of David Sherrington. I have known David for most of his career and *all* of mine, since he was the external examiner for my D. Phil. viva in 1973. Subsequently we were colleagues at Imperial College for several years, and David hosted my sabbatical in Oxford in 2001–02. In addition, we have had many discussions on spin glasses over the years.

Spin glasses are systems with two key ingredients: *disorder*, and *frustration*, i.e. competition between different terms in the Hamiltonian so they cannot all be satisfied simultaneously. Figure 1 shows a toy example of frustration with a single square of Ising spins. (Ising spins can only point up or down.) The '+' or '−' on the bonds indicates a ferromagnetic or antiferromagnetic interaction, respectively. In this example, with one negative bond, it is impossible to minimize the energy of all the bonds so there is competition or 'frustration'.

Most theoretical work therefore uses the simplest model with the features of disorder and frustration, the Edwards Anderson [1] (EA) model, whose Hamiltonian is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i h_i S_i. \tag{1}$$
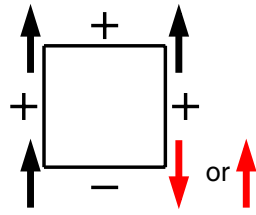
Figure 1. A toy model which shows frustration. If the interaction on the bond is a '+', the spins want to be parallel and if it is a '−' they want to be antiparallel. Clearly all these conditions cannot be met simultaneously so there is competition or 'frustration'.

The Ising spins S_i take values ± 1 and lie on the sites i of a three-dimensional, simple cubic lattice with $N = L^3$ sites. Periodic boundary conditions are applied. The interactions J_{ij} are between nearest neighbors and are independent random variables with a symmetric distribution and standard deviation unity, i.e.

$$[J_{ij}]_{\mathrm{av}} \equiv J_0 = 0; \qquad [J_{ij}^2]_{\mathrm{av}}^{1/2} \equiv J = 1, \tag{2}$$

where $[\cdots]_{\mathrm{av}}$ means an average over the disorder. We will also use the notation $\langle\cdots\rangle$ to indicate a thermal average for a particular set of interactions. The precise form of the distribution of J_{ij} is not very important but, for technical reasons, it will be convenient to take a Gaussian distribution in the simulations reported here. In some of what follows we shall also include a magnetic field h_i.

Motivated by the pioneering work of Edwards and Anderson [1] (EA), David, together with Scott Kirkpatrick, [2] (SK) proposed that the mean-field theory of spin glasses should be the exact solution of an infinite-range version of the EA model in which there is no lattice and the distribution of the J_{ij} is the *same* for all distinct pairs i and j. In order to get a sensible thermodynamic limit, one has to scale the variance of the distribution by N, i.e. $[J_{ij}^2]_{\mathrm{av}}^{1/2} = 1/\sqrt{N}$.

The SK solution of their model was of the same type as that found by EA, what we now call the 'replica symmetric' (RS) solution. Perhaps the most important advance in the SK paper, relative to EA, is that SK realized that *the RS solution cannot be correct* since the entropy went negative at low temperatures (which is impossible for an Ising model since the states can be counted).

Almeida and Thouless [3] subsequently clarified what was going wrong. They looked at the stability of the RS solution in the magnetic field–temperature plane. They found that the RS solution was stable above a line in this plane, see figure 2, but was unstable below this line.

The theory used the 'replica trick' in which averages over the quenched disorder are carried out by making n copies ('replicas') of the system and letting n tend to zero. In the RS solution, all pairs of replicas are equivalent and there is a single-order parameter. It was clear that this 'replica symmetry' had to be broken below the AT line but how to do so was not obvious, since the size of the space, n, is non-integer and tends to zero. In a tour-de-force, Parisi [4, 5] proposed a hierarchical 'replica symmetry breaking' (RSB) solution with an infinite number of parameters. Twenty-seven years after Parisi introduced his solution, its free energy was rigorously proved to be exact by Tallegrand [6].

The Parisi solution has two important features:

- The first, as we have seen, is that there is line of phase transitions in a magnetic field (AT line).
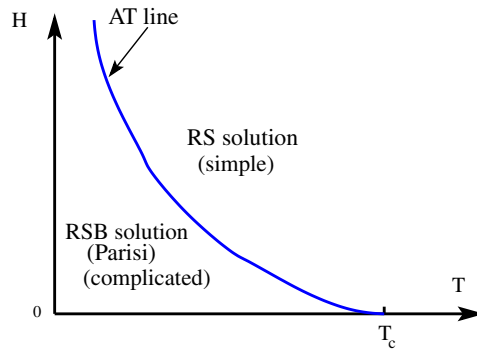
Figure 2. The magnetic field–temperature phase diagram of the SK model according to Almeida and Thouless [3]. Above the line, the replica symmetric solution of SK is correct, while below the line one has to break the symmetry in a more complicated way, i.e. the 'replica symmetry breaking' (RSB) solution of Parisi.

- The second is that below the AT line the order parameter is not just a single number but a *function* (actually a probability distribution), i.e. there are an infinite number of order parameters. The theory involves the overlap between two spin configurations, q, defined by

$$q = \frac{1}{N} \sum_{i=1}^{N} S_i^{(1)} S_i^{(2)}, \tag{3}$$

where (1) and (2) refer to two (real) copies of the system with the same interactions. Below the AT line, q has a non-trivial distribution $P(q)$, which, for zero field, looks as in figure 3.

As soon as the field becomes non-zero the negative-q region is eliminated because the symmetry is now broken (one of the two states which were related by time-reversal symmetry in the zero field is suppressed), and there is a non-zero weight in the distribution between q_{EA} (which turns out to be only very weakly dependent on field) and q_{min} where $0 < q_{min} < q_{EA}$. As the AT line is approached from below q_{min} tends to q_{EA}, and above the AT line the distribution is just a delta function at q_{EA}. This is the replica symmetric solution.

The motivations for SK to introduce their infinite-range model were (i) it should be exactly solvable and (ii) the behavior of real spin glasses might have similar features to the exact solution. We have seen that (i) is correct, though the exact solution was harder to find than expected. Whether (ii) is a correct has been, and continues to be, controversial.

The hypothesis that real spin glasses behave in a similar way to the SK model is called the RSB scenario for the spin glass state. Another scenario, with different predictions, has also been proposed called the 'droplet picture'. This was developed in most detail by Fisher and Huse [7–9], though similar ideas were also proposed by Bray and Moore [10] and McMillan [11]. The droplet picture differs from the RSB scenario in two important respects: (i) there is no AT line and (ii) the order parameter is just a single number q_{EA}, since the distribution $P(q)$ is just two delta functions (in zero field) at $q = \pm q_{EA}$, i.e. the continuous 'non-trivial' part in figure 3 is missing.

In the rest of this paper, I will use numerical simulations to ascertain whether the RSB or droplet picture (or neither) is correct. In section 2, I discuss the finite-size scaling method used
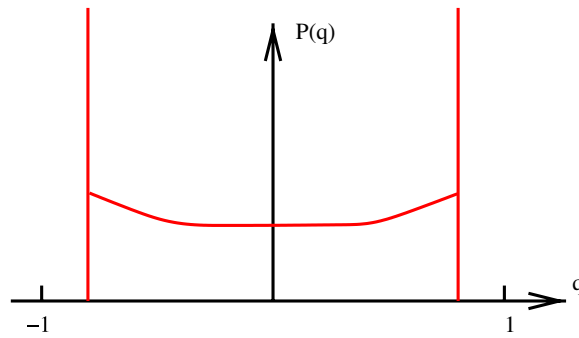
Figure 3. The order parameter distribution in the Parisi field for $h = 0$. Note that it is symmetric because of time-reversal symmetry. There is a delta function at $q = q_{EA}$ where the two copies are in the same valley (and one at $-q_{EA}$ where one copy is the time-reversed image of the other). There is also a 'non-trivial' part *with a non-zero weight even at $q = 0$*, where the two copies are in different valleys.

to analyze the data, and in section 3 I describe the parallel tempering Monte Carlo method which speeds up equilibration at low temperature. In addition to the short-range EA model in three dimensions described above, it will also be useful to consider a one-dimensional model with long-range interactions. This is discussed in section 4. Results for the order parameter distribution are discussed in section 5 and results concerning the existence of an AT line are discussed in section 6. Finally, the conclusions are summarized in section 7.

2. Finite-size scaling

In the later sections we will use numerical simulations to investigate phase transitions in spin glasses. Of course, a sharp transition can only occur in the thermodynamic limit, whereas simulations are carried out on finite-size lattices. We therefore use the technique of finite-size scaling (FSS) to extrapolate from results on a *range* of finite sizes to the thermodynamic limit. Following Ballesteros *et al* [12], we shall find the correlation length of the finite system to be a particularly useful quantity to analyze by FSS.

To extract a correlation length we define the spin glass susceptibility at finite wavevector **k**

$$\chi_{SG}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} [\langle S_i S_j \rangle^2]_{av} \, e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \tag{4}$$

We then determine the finite-size spin glass correlation length ξ_L from the Ornstein–Zernicke equation:

$$\chi_{SG}(\mathbf{k}) = \frac{\chi_{SG}(\mathbf{0})}{1 + \xi_L^2 \mathbf{k}^2 + \cdots}, \tag{5}$$

by fitting to $\mathbf{k} = 0$ and $\mathbf{k} = \mathbf{k}_{min} = \frac{2\pi}{L}(1, 0, 0)$.

The basic assumption in FSS is that the size dependence of the results comes from the ratio L/ξ_{bulk} where

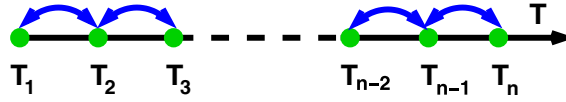$$\xi_{bulk} \sim (T - T_{SG})^{-\nu} \tag{6}$$

Figure 4. Sketch illustrating the temperature swaps in the parallel tempering method.

is the *bulk* (i.e. infinite-system size) correlation length. In particular, the correlation length ξ_L of the simulated system, which has linear size L, varies as

$$\frac{\xi_L}{L} = X(L^{1/\nu}(T - T_{SG})). \tag{7}$$

Since ξ_L/L is dimensionless it turns out that there is no power of L multiplying the scaling function X. This is very useful because, according to equation (7), data for different sizes *intersect* at T_{SG}. Hence the transition temperatures can be determined by eye. Furthermore, if there is a long-range spin glass order then the data should splay out below T_{SG}. This works very well for the Ising spin glass [12, 13]

If we had used χ_{SG}, rather than ξ_L as the quantity to analyze, there would have been an additional factor of L to an unknown power multiplying the scaling function in equation (7) which would have complicated the analysis.

3. Parallel tempering

Experimentally, spin glass dynamics becomes very slow at low temperatures, because the system has a very complicated 'energy landscape' with many 'valleys', separated by barriers, in which the system gets trapped. In Monte Carlo simulations too, the system gets trapped in a valley at low temperature, and conventional Monte Carlo simulations take a huge amount of time to equilibrate in this region. Most Monte Carlo simulations of spin glasses, including those described here, therefore use a modified approach known as parallel tempering (replica exchange) [14], which helps the system get over barriers and equilibrate at low temperature. This approach, which I now describe, is of quite general applicability to problems with a complicated energy landscape.

One simulates a copy of the system, with the same interactions, at each of n temperatures between $T_{\min} = T_1$ and $T_{\max} = T_n$, see figure 4. The highest temperature is chosen so that the system equilibrates fast; it has enough energy to easily get over the barriers. The lowest temperature is chosen in the region one wants to study. In addition to the usual single-spin updates at each temperature, one also performs temperature swaps in which the entire spin configurations at neighboring temperatures, T_l and T_{l+1}, are swapped with probability

$$P_{\mathrm{swap}} = \exp[(\beta_l - \beta_{l+1})(E_l - E_{l+1})], \tag{8}$$

where $\beta_l = 1/T_l$, and E_l is the *total* energy of the copy at temperature T_l. It is not difficult to check that equation (8) satisfies the detailed balance condition, and so eventually the whole set of copies will come to thermal equilibrium.

The price one pays is that one has to simulate several (sometimes many) copies of the system. Not all this is wasted, though, since one usually does want results at several temperatures. However, there is an overhead because one ends up doing more sweeps than necessary at high temperatures, and quite often one is forced to use more temperatures than are really needed. This is particularly the case for large sizes because the spacing between
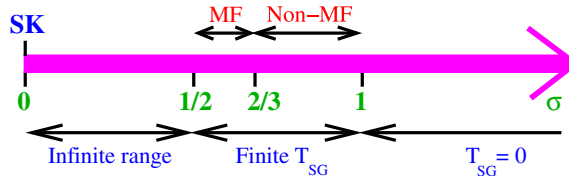
Figure 5. The different types of behavior of the long-range model in $d = 1$ as a function of the power σ with which the interactions fall off with distance.

temperatures has to vary with N as $N^{-1/2}$, so the number of temperatures varies as $N^{1/2}$, in order that the probability in equation (8) is significant. Physically this is because the same spin configuration must be one which occurs with significant probability at *both* T_l and T_{l+1}. However, at low temperature, one finds that the speed up of the relaxation time more than compensates for the overhead in simulating a large number of temperatures.

4. Model with long-range interactions

For short-range models, there is a *lower critical dimension* d_l (equal to [15] about 2.5), below which the finite-temperature zero-field transition disappears, and *an upper critical dimension* d_l (equal to 6) where the zero-field transition is described by mean-field exponents, i.e. those of the EA–SK theory.

It is therefore of interest to investigate spin glasses not only in three dimensions but also in higher dimensions. Even with parallel tempering it is difficult to equilibrate more than of order a thousand spins at low temperatures, and since $N = L^d$ the range of L is very limited at high d. We will therefore also consider a one-dimensional model in which the interactions fall off with a power of the distance:

$$J_{ij} \propto \frac{\epsilon_{ij}}{r_{ij}^{\sigma}}, \qquad [\epsilon_{ij}]_{\mathrm{av}} = 0, \qquad [\epsilon_{ij}^2]_{\mathrm{av}} = 1. \qquad (9)$$

For each σ we rescale the interactions so that the mean-field transition temperature T_{SG}^{MF} is unity (for zero field).

This model is useful because one can make an analogy between varying d for short-range models, and varying σ for the long-range model in $d = 1$. This has been well established for ferromagnets, e.g. [16]. In particular there is a σ_l *above* which $T_{SG} = 0$, and a σ_u *below* which the zero-field critical behavior is mean-field-like, where $\sigma_l = 1$ [9] and $\sigma_u = 2/3$ [17]. Note too that $\sigma = 0$ is the SK model and the range $0 \leqslant \sigma \leqslant 1/2$ is *infinite-range* since $\sum_j [J_{ij}^2]_{\mathrm{av}}$ diverges. Furthermore, $\sigma \to \infty$ is the nearest-neighbor model. Figure 5 summarizes the behavior of the $d = 1$ long-range model as a function of σ.

5. Results for the order parameter distribution $P(q)$

In this section we consider only the zero magnetic field.

As discussed in section 1, the RSB picture of the spin glass state below T_{SG} predicts that the order parameter distribution $P(q)$ should have a continuous part with a finite weight even at $q = 0$. By contrast the droplet theory predicts that the weight in the continuous part should be zero in the thermodynamic limit. More precisely, the prediction is [7] that $P(0) \propto 1/L^\theta$ where $\theta (>0)$ is a stiffness exponent, estimated to be about 0.20 [20, 21] for the Ising spin glass in three dimensions.
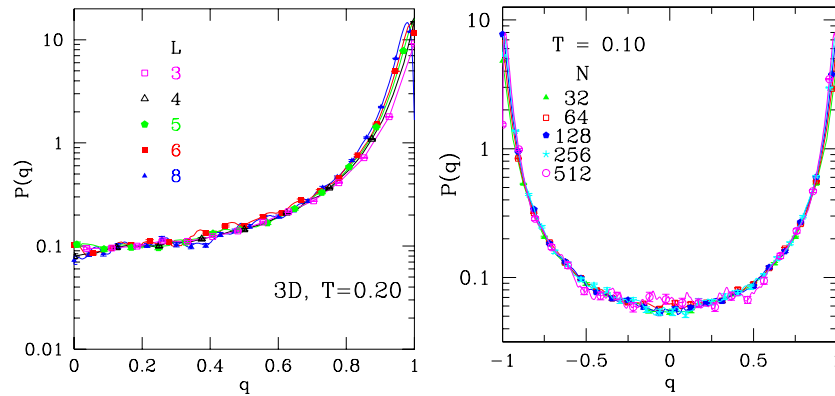
Figure 6. The left-hand figure is the order parameter distribution in the zero field for the short-range model in $d = 3$ at $T = 0.20$ which is to be compared with the transition temperature of $T_{SG} \simeq 0.95$ [13] (from Katzgraber *et al* [18]). The right-hand figure is for the long-range model with $\sigma = 0.75$, which is in the nonmean-field, finite T_{SG} region, see figure 5. The temperature is $T = 0.10$ which is to be compared with the mean-field transition temperature of 1, and the actual transition temperature of about 0.62. (From Katzgraber and APY [19].)

The left-hand side of figure 6, from [18], shows that $P(0)$ is independent of size for $3 \leqslant L \leqslant 8$ at a temperature of 0.20, far below the transition temperature of about 0.95. The right-hand side of this figure shows similar data, from [19], for the long-range model with $\sigma = 0.75$, in the region predicted to have a finite transition temperature with nonmean-field exponents. The temperature is 0.10 compared with the transition temperature of about 0.62. The stiffness exponent is expected to be [9] $d - \sigma = 0.25$. For a large range of sizes, $32 \leqslant L \leqslant 512$, one again finds that $P(0)$ is independent of size.

For the range of sizes that can be studied, which is quite large for the 1D model, we see that the data for $P(q)$ are consistent with the RSB picture and inconsistent with the droplet picture. Of course, it is possible that the sizes are too small to see the asymptotic critical behavior. However, if the droplet theory is correct asymptotically, one would need extremely large sizes to see it, especially for the 1D model.

6. Ising spin glass in a magnetic field

As discussed in section 1, in the SK model there is a line of phase transitions in a magnetic field for an Ising spin glass, known as the Almeida Thouless [3] (AT) line, which separates a spin glass phase, with divergent relaxation times and 'replica symmetry breaking', from a paramagnetic 'replica symmetric' phase with finite relaxation times, see figure 2. Experimentally, it is harder to determine whether there is an AT line than whether there is a transition in the zero field. The reason is that the experimentally measurable nonlinear susceptibility, χ_{nl}, diverges in the zero field, providing a clear signature of the transition, whereas χ_{nl} does *not* diverge on the AT line at the non-zero field. Experiments therefore look for another signature of the transition, a divergent relaxation time. In a careful experiment [22], *no* such divergence in a field was found, implying the absence of an AT line. However, not all experiments have come to the same conclusion.
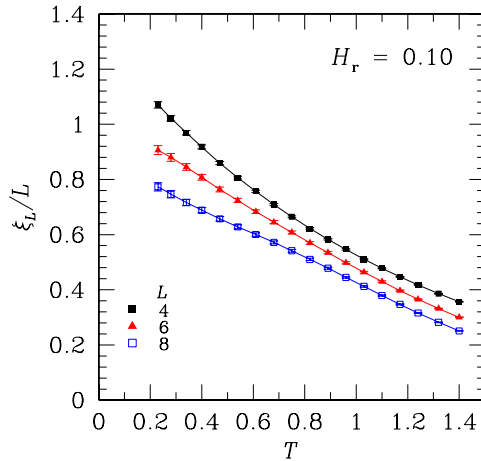
Figure 7. The scaled correlation length for the Ising spin glass with (random) field strength $H_r = 0.1$ (Katzgraber and Young, unpublished).

Although there is no static divergent quantity measurable in *experiments*, there *is* such a quantity which is accessible in *simulations*, namely the spin glass susceptibility χ_{SG}. The zero-field definition of χ_{SG} given in equation (4) is generalized in a field to

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

Equation (10) is just the 'replicon mode' of replica field theory, which diverges for the SK model along the AT line. More conveniently, one can obtain from the simulations a correlation length ξ_L from $\chi_{SG}(\mathbf{k})$ using equation (5), and this can be analyzed by FSS according to equation (7), so the transition is indicated by intersection of the data for different sizes.

In the simulations [24] we actually used a Gaussian random field, rather than a uniform field, for technical reasons, but MFT predicts an AT line for this case too, just as for a uniform field. Some results are shown in figure 7 for the three-dimensional, nearest-neighbor model. The strength of the (random) field is $H_r = 0.1$ which is very small compared with the zero-field transition temperature [13] $T_{SG} \simeq 0.96$. There is no intersection, which indicates that there is no AT line.

Subsequently, we [23] looked for the AT line in the 1D model with long-range interactions described in section 4, and some data are shown in figure 8. One sees a clear intersection, indicating a transition in a field, i.e. an AT line, for $\sigma = 0.55$, which is in the mean-field regime. For $\sigma = 0.75$ and 0.85, which are in the non mean-field region, no AT line is seen. For the other value of σ presented, 0.65, which is close to the borderline value (2/3) between the mean-field and nonmean-field regions, there *are* intersections at low T for the smaller sizes, but the data for $L = 128$ and 256 merge at low T indicating marginal behavior. The data for $L = 512$ appear slightly higher at the lowest T which could be equilibrated, but the difference is only about the same as the error bars.

Hence the data are consistent with there being an AT line in the region where the zero-field transition is mean-field-like. For the short-range case this would be $d > 6$. (I emphasize that we are not able to simulate *directly* the spin glass in a field for $d > 6$, and this conclusion is obtained *by analogy* with the 1D model with long-range interactions.)
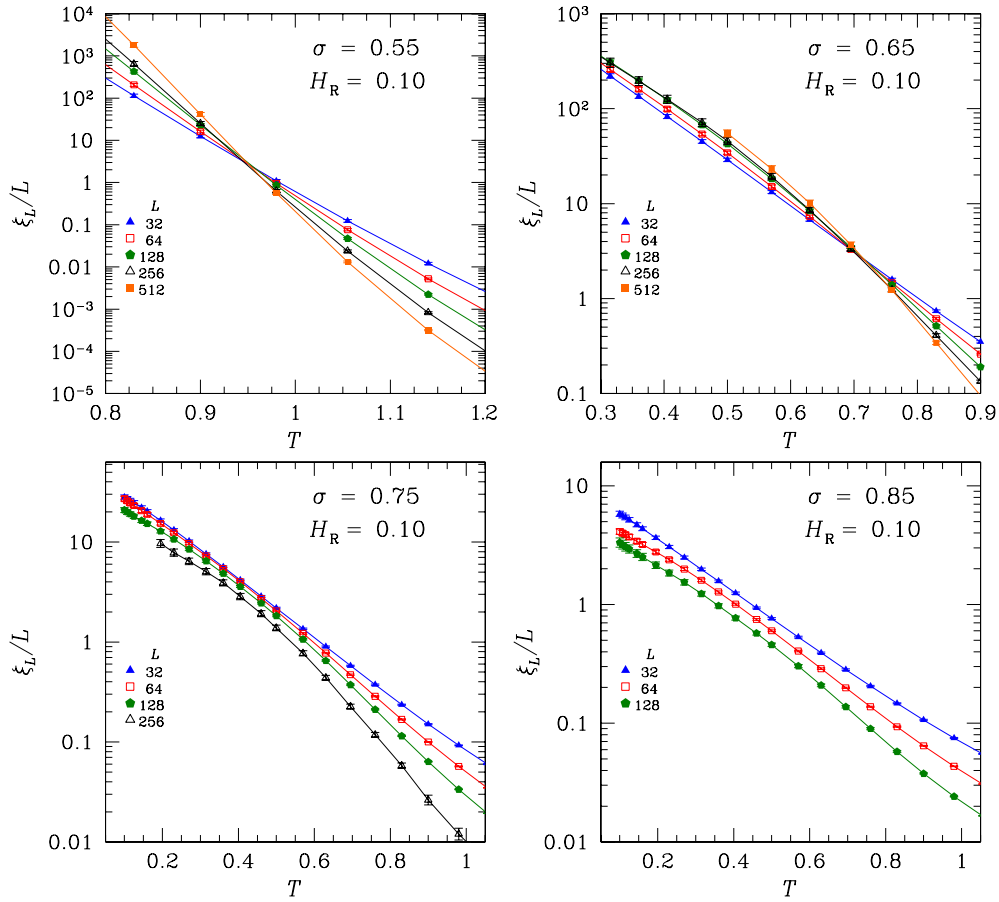
Figure 8. Data for the scaled correlation length of the one-dimensional model with long-range interactions in a magnetic field from [23]. Results are presented for $\sigma = 0.55$, which is in the mean-field regime (for the zero-field transition), see figure 5, $\sigma = 0.65$, which is close to the borderline between the mean-field and nonmean-field regions, and $\sigma = 0.75$ and 0.85, which are in the nonmean-field region. One sees an intersection, indicating a transition in a field, i.e. an AT line, only for $\sigma = 0, 55$. The case of $\sigma = 0.65$ seems to be borderline, as discussed in the text.

7. Conclusions

The question we posed in this paper is whether the Sherrington–Kirkpatrick model is relevant for real spin glasses. Taken literally, the numerical results indicate that for $d > 6$ the answer is 'yes' while for $3 \leqslant d < 6$ the answer is 'only partly'. For the latter case, the data for $P(q)$ are consistent with the RSB picture (i.e. with the behavior of the SK model) while the absence of an AT line disagrees with the RSB picture. The numerical data for $d < 6$ thus favor an intermediate scenario, called 'TNT' by Krzakala and Martin [25], see also [26].

However, it is possible that the numerical data are not in the asymptotic regime, and the devotees of the droplet picture claim that it does hold asymptotically (at least for $d < 6$). If this is so, then it must only apply for quite large lattice sizes, (especially for the analogous one-dimensional model).

Acknowledgments

References

[1] Edwards S F and Anderson P W 1975 *J. Phys. F* **5** 965
[2] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792
[3] de Almeida J R L and Thouless D J 1978 *J. Phys. A: Math. Gen.* **11** 983
[4] Parisi G 1979 *Phys. Rev. Lett.* **43** 1754
[5] Parisi G 1980 *J. Phys. A: Math. Gen.* **13** 1101
[6] Talagrand M 2006 *Ann. Math.* **163** 221
[7] Fisher D S and Huse D A 1986 *Phys. Rev. Lett.* **56** 1601
[8] Huse D A and Fisher D S 1987 *J. Phys. A: Math. Gen.* **20** L997
[9] Fisher D S and Huse D A 1988 *Phys. Rev. B* **38** 386
[10] Bray A J and Moore M A 1986 *Heidelberg Colloquium on Glassy Dynamics and Optimization* ed L Van Hemmen and I Morgenstern (Berlin: Springer) p 121
[11] McMillan W L 1984 *J. Phys. A: Math. Gen.* **17** 3179
[12] Ballesteros H G, Cruz A, Fernandez L A, Martin-Mayor V, Pech J, Ruiz-Lorenzo J J, Tarancon A, Tellez P, Ullod C L and Ungil C 2000 *Phys. Rev. B* **62** 14237 (*Preprint* cond-mat/0006211)
[13] Katzgraber H G, Körner M and Young A P 2006 *Phys. Rev. B* **73** 224432 (*Preprint* cond-mat/0602212)
[14] Hukushima K and Nemoto K 1996 *J. Phys. Soc. Japan* **65** 1604
[15] Boettcher S 2005 *Phys. Rev. Lett.* **95** 197205
[16] Fisher M E, Ma S k and Nickel B G 1972 *Phys. Rev. Lett.* **29** 917–20
[17] Kotliar G, Anderson P W and Stein D L 1983 *Phys. Rev. B* **27** 602
[18] Katzgraber H G, Palassini M and Young A P 2001 *Phys. Rev. B* **63** 184422 (*Preprint* cond-mat/0108320)
[19] Katzgraber H G and Young A P 2003 *Phys. Rev. B* **67** 134410 (*Preprint* cond-mat/0210451)
[20] Hartmann A K 1999 *Phys. Rev. E* **59** 84
[21] Boettcher S 2004 *Eur. Phys. J. B* **38** 83
[22] Mattsson J, Jonsson T, Nordblad P, Katori H A and Ito A 1995 *Phys. Rev. Lett.* **74** 4305
[23] Katzgraber H G and Young A P 2005 *Phys. Rev. B* **72** 184416 (*Preprint* cond-mat/0407031)
[24] Young A P and Katzgraber H G 2004 *Phys. Rev. Lett.* **93** 207203 (*Preprint* cond-mat/0407031)
[25] Krzakala F and Martin O C 2000 *Phys. Rev. Lett.* **85** 3013 (*Preprint* cond-mat/0002055)
[26] Palassini M and Young A P 2000 *Phys. Rev. Lett.* **85** 3017 (*Preprint* cond-mat/0002134)