Ising Spin-Glass Transition in a Magnetic Field Outside the Limit of Validity of Mean-Field Theory

L. Leuzzi,[1,2] G. Parisi,[1,2,3] F. Ricci-Tersenghi,[1,3] and J. J. Ruiz-Lorenzo[4]

[1]*Dipartimento di Fisica, Sapienza Università di Roma, P.le Aldo Moro 2, I-00185 Roma, Italy*
[2]*Statistical Mechanics and Complexity Center (SMC) - INFM - CNR, Roma, Italy*
[3]*INFN - Sezione di Roma1, Sapienza Università di Roma, P.le Aldo Moro 2, I-00185 Roma, Italy*
[4]*Departamento de Física, Univ. Extremadura, Badajoz, E-06071 and BIFI, Spain*

(Received 3 December 2008; revised manuscript received 15 September 2009; published 22 December 2009)

The spin-glass transition in a magnetic field is studied both in and out of the limit of validity of mean-field theory on a diluted one dimensional chain of Ising spins where exchange bonds occur with a probability decaying as the inverse power of the distance. Varying the power in this long-range model corresponds, in a one-to-one relationship, to changing the dimension in spin-glass short-range models. Evidence for a spin-glass transition in a magnetic field is found also for systems whose equivalent dimension is below the upper critical dimension in a zero magnetic field.

DOI: 10.1103/PhysRevLett.103.267201 PACS numbers: 75.10.Nr, 05.70.Fh, 71.55.Jv

Introduction.—Even though 30 years have passed since the spin-glass (SG) phase in the presence of an external magnetic field has been characterized in mean-field (MF) theory [1], its existence in realistic finite-dimensional systems is not yet established. In most common (Heisenberg-like) SG alloys, e.g., AgMn, CuMn, and AuFe, a SG phase has been detected also in the presence of an external field [2]. In the MF theory of vectorial SG this transition is expected along the so-called Gabay-Toulouse line [3]. In Ising-like materials, instead, like $Fe_xMn_{1-x}TiO_3$, it is still a matter of debate whether or not a SG phase occurs when the system is embedded in a magnetic field [2,4]. Irreversible phenomena are, actually, detected in experiments as the temperature is lowered: the separation of zero-field cooled and field-cooled susceptibilities (or magnetizations) and the rapid increase of characteristic relaxation times. In a zero field these are the signatures of a thermodynamic transition, but in some recent ac measurements in a magnetic field [4], their magnitude tends to depend sensitively on frequency and they are interpreted as pertaining to a glassy dynamic arrest, rather than to a true thermodynamic transition. According to this, the SG features measured in a field would be artifacts of being out of equilibrium, similar to what happens in the structural glass transition, in which the liquid glass former falls out of equilibrium at low T when its structural relaxation time becomes longer than the observation time and it vitrifies into an amorphous solid.

The replica symmetry breaking theory, holding in the MF regime for SG, predicts a thermodynamic transition in magnetic field h at a finite temperature [5]. In this framework, a transition line, called the de Almeida–Thouless (dAT) [1] line, can be identified in the T-h plane between a paramagnetic and a SG phase. At sufficiently low dimensions (i.e., below the lower critical dimension, D_L) the transition disappears. The value of D_L is not known, but it is quite possible that in a field D_L is higher than for $h = 0$ (as it happens for a ferromagnet in a random field). There are numerical evidences and analytic results [6] supporting $D_L = 2.5$ at zero field. For $h > 0$, some arguments suggested $D_L = 6$, but recently Temesvari [7] argued that the dAT line can be continued below $D = 6$. In the droplet theory, instead, no transition is predicted to remain as soon as an infinitesimal field is switched on, independently from the value of D. A crossover length $\ell_d(h, T)$ is introduced [8], beyond which the SG phase is destroyed by the field. The predictions of the trivial-non-trivial scenario [9] should be similar to those of the droplet model. Extensive numerical works on the Edwards-Anderson model in 4D and 3D yielded evidence both in favor of a transition in field [10,11] and against it [12–14]. Unfortunately, finite size corrections are very strong in the presence of an external field and it is hard to say whether these simulations were really testing the thermodynamic limit. To overcome this problem we use a recently introduced SG model [15], which can be simulated very efficiently, and a new data analysis, which should be less sensitive to finite size effects (FSE). We report numerical evidences for a phase transition in the presence of external fields also in systems for which the MF approximation is not correct.

The model.—We investigate a one dimensional chain of L Ising spins ($\sigma_i = \pm 1$) whose Hamiltonian reads [15]

$$\mathcal{H} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i. \quad (1)$$

The quenched random couplings J_{ij} are independent and identically distributed random variables taking a nonzero value with a probability decaying with the distance between spins σ_i and σ_j, $r_{ij} \equiv \min(|i-j|, L-|i-j|)$, as

$$\mathbf{P}[J_{ij} \neq 0] \propto r_{ij}^{-\rho} \quad \text{for } r_{ij} \gg 1. \quad (2)$$

Nonzero couplings take the value ± 1 with equal probability. We use periodic boundary conditions and a $z = 6$

average coordination number [16]. The random field h_i is Gaussian distributed with zero average and standard deviation h [17]. We will denote the average over quenched disorder (bonds and fields) by an overline. The universality class depends on the value of ρ. For $\rho > 1$ it turns out to be equal to the one of the fully connected version of the model [18], where bonds are Gaussian distributed with zero mean and a variance depending on the distance as $\overline{J_{ij}^2} \propto r_{ij}^{-\rho}$. As ρ varies, the model displays different behaviors [15]: for $\rho \leq \rho_U \equiv 4/3$, the MF approximation is exact, while for $\rho > \rho_U$, it breaks down because of infrared divergences (IRD). The value $\rho_U = 4/3$ corresponds to the upper critical dimension (UCD) of short-range SG in the absence of an external magnetic field ($D_U = 6$). At $\rho > \rho_L = 2$ no finite temperature transition occurs, even for $h = 0$ [19]. A relationship between ρ and the dimension D of short-range models can be expressed as $\rho = 1 + 2/D$ which is exact at $D_U = 6$ ($\rho_U = 4/3$) and *approximated* as $D < D_U$ [20]. We note that in the ferromagnetic (ordered) Ising case on the same kind of lattices, a simple theoretical argument tells us that the value of ρ_L is 2 for $h = 0$ and 1.5 in a field.

Simulations details and data analysis.—We simulated two replicas $\sigma_i^{(1,2)}$ using the parallel tempering algorithm [21]. Field values are $h = 0, 0.1, 0.2, 0.3$ for $\rho = 0, 1.2, 1.4$ and $h = 0, 0.1, 0.15, 0.2$ for $\rho = 1.5$. We used sizes up to $L = 2^{14}$ spins for $h = 0$ and up to $L = 2^{12}$ for $h > 0$. The number of samples is between 32 000 and 64 000 for all sizes. Thermalization is guaranteed by the logarithmic binning (in base 2) of data in MC steps until at least the last two points coincide.

The presence of the SG long range order can be deduced from the study of the four-point correlation function [22]

$$C(x) = \sum_{i=1}^{L} \overline{(\langle\sigma_i \sigma_{i+x}\rangle - \langle\sigma_i\rangle\langle\sigma_{i+x}\rangle)^2} \tag{3}$$

and its Fourier transform $\tilde{C}(k)$. Indeed, both the SG susceptibility

$$\chi_{\rm sg} \equiv \tilde{C}(0) \tag{4}$$

and the so-called second-moment correlation length [23]

$$\xi \equiv \frac{1}{2\sin(\pi/L)}\left[\frac{\tilde{C}(0)}{\tilde{C}(2\pi/L)} - 1\right]^{1/\rho-1} \tag{5}$$

diverge at the critical temperature in the thermodynamic limit. For finite (but large enough) systems, the following scaling laws hold in the MF regime ($1 < \rho \leq 4/3$)

$$\frac{\chi_{\rm sg}}{L^{1/3}} = \tilde{\chi}[L^{1/3}(T - T_c)], \quad \frac{\xi}{L^{\nu/3}} = \tilde{\xi}[L^{1/3}(T - T_c)] \tag{6}$$

with $\nu = 1/(\rho - 1)$, and in the IRD regime ($\rho > 4/3$)

$$\frac{\chi_{\rm sg}}{L^{2-\eta}} = \tilde{\chi}[L^{1/\nu}(T - T_c)], \quad \frac{\xi}{L} = \tilde{\xi}[L^{1/\nu}(T - T_c)]. \tag{7}$$

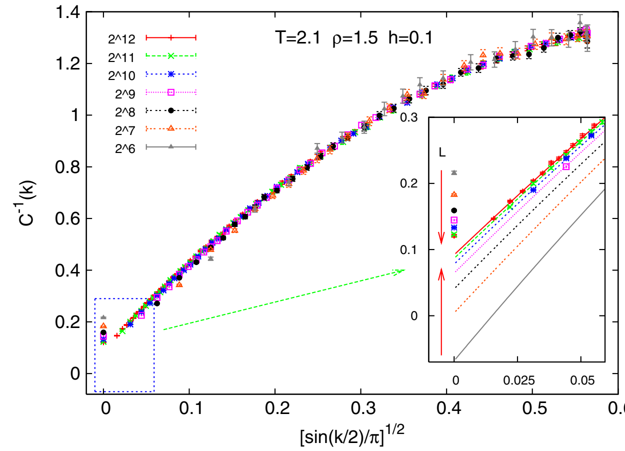

FIG. 1 (color online). $\tilde{C}(k)^{-1}$ vs $\sqrt{\sin(k/2)/\pi}$ at $\rho = 1.5$ (IRD regime), $h = 0.1$, $T = 2.1$ and $L = 2^6, \ldots, 2^{12}$. Inset: comparison between $\tilde{C}(0)^{-1}$ and its extrapolated valued A.

with $2 - \eta = \rho - 1$ [18]. Unfortunately, finite size corrections to the above scaling laws are known to be very large, especially in the presence of an external field. It is very important to understand these FSE and try to keep them under control. In the main panel of Fig. 1 we plot $1/\tilde{C}(k)$ versus $[\sin(k/2)/\pi]^{\rho-1}$ for an interesting case (IRD regime with field). For $L \rightarrow \infty$ and $T > T_c$ the propagator on the lattice at small wave numbers should behave like

$$\tilde{C}(k)^{-1} \simeq A + B[\sin(k/2)]^{\rho-1}, \tag{8}$$

with $\chi_{\rm sg} = 1/A$ and $\xi \propto (B/A)^{1/(\rho-1)} = (B\chi_{\rm sg})^{1/(\rho-1)}$. In other words, $A(L = \infty, T)$ goes to zero at T_c, while $B(L = \infty, T = T_c)$ stays finite.

We observe in Fig. 1 that the largest FSE in $\tilde{C}(k)$ are in $k = 0$, which are the data used for estimating $\chi_{\rm sg}$. Moreover, FSE for $k > 0$ have an opposite sign with respect to those in $k = 0$ (cf. lower inset) and consequently ξ, which is a function of $\tilde{C}(0)/\tilde{C}(2\pi/L)$, may be strongly

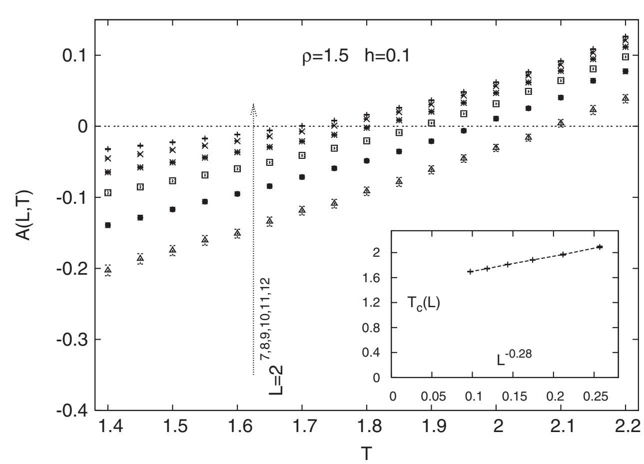

FIG. 2. Plot of $A(L, T)$ vs T at $\rho = 1.5$, $h = 0.1$. Sizes are $L = 2^7, \ldots, 2^{12}$. Inset: $T_c(L)$ vs $L^{-0.28}$.

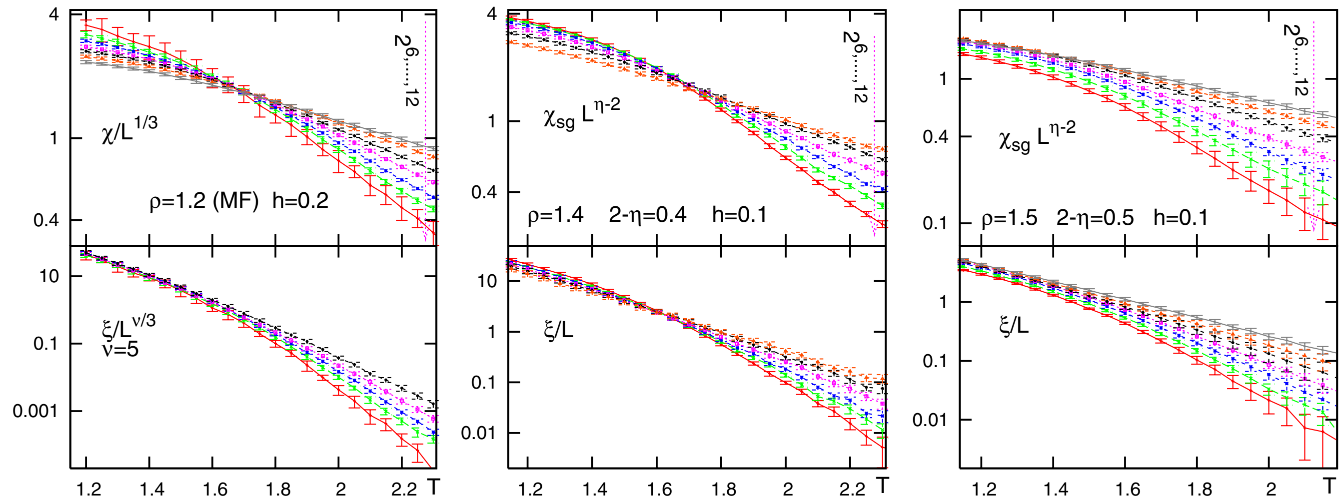

FIG. 3 (color online). Scaling functions vs T. Left panels: $\rho = 1.2$, $\chi_{\rm sg}/L^{1/3}$ (top) and $\xi/L^{5/3}$ (bottom) at $h = 0.2$. Sizes are $L = 2^6, \ldots, 2^{12}$. Mid panels: $\rho = 1.4$, $\chi_{\rm sg}/L^{0.4}$ and ξ/L at $h = 0.1$. Lower panels: $\rho = 1.5$, $\chi_{\rm sg}/L^{0.5}$ and ξ/L at $h = 0.1$.

affected. FSE are more evident in the large x tail of $C(x)$ and, thus, at small k in $\tilde{C}(k)$, while they decrease as k increases. The large x part of $C(x)$ strongly depends on the average overlap order parameter $\overline{\langle q \rangle}$, which is known to have strong sample-to-sample fluctuations in a field and FSE due to negative overlaps which should disappear in the thermodynamic limit.

With the aim of reducing FSE, we introduce a method for estimating T_c using $\tilde{C}(k)$ data with $k > 0$. We fit $\tilde{C}(k)^{-1}$ by a quadratic function $A + By + Cy^2$ with $y = [\sin(k/2)/\pi]^{\rho-1}$: the resulting fits have a $\chi^2/\text{d.o.f.} < 0.55$ (comparable fit qualities have been found in the entire analysis). As long as $T > T_c$, we expect $\lim_{L\to\infty} A(L, T) = \chi_{\rm sg}^{-1} > 0$: the inset in Fig. 1 shows the size dependence of $\tilde{C}(0)^{-1}$ and $A(L, T)$, with compatible $L \to \infty$ limits.

In Fig. 2 we show the best fitting parameter $A(L, T)$ for $\rho = 1.5$ and $h = 0.1$. For each size we compute the temperature $T_c(L)$ by solving the equation $A(L, T_c(L)) = 0$ (in this way only $A > 0$ data are used, which are the most reliable). Finally, we estimate $T_c = \lim_{L\to\infty} T_c(L)$ (inset of Fig. 2) and obtain $T_c = 1.46(3)$. The $T_c(L)$ scaling in $L^{-1/\nu}$ has an exponent -0.28, in good agreement with $1/\nu = 0.25(3)$ for the $h = 0$ case [15]. On the same data ($\rho = 1.5$, $h = 0.1$) the analysis of the crossing points of $\chi_{\rm sg}/L^{2-\eta}$ and ξ/L, cf. Eq. (7), is shown in Fig. 3 (right panel), yielding no evidence for a phase transition, as in Ref. [24]. A very natural explanation is the presence of strong corrections to Eq. (7). The case $\rho = 1.4$, $h = 0.1$, provides a still more useful comparison. Our method returns a critical temperature $T_c = 1.67(7)$. Figure 3 shows $\chi_{\rm sg}/L^{2-\eta}$ and ξ/L vs T: crossings are present, but the curves seem to merge for $T \lesssim 1.5$ and a precise determination of T_c is practically unfeasible. For $\rho = 1.2$, $h = 0.2$, the estimate based on the scaling of $\chi_{\rm sg}/L^{1/3}$, Eq. (6), yields $T_c = 1.67(3)$, while $\xi/L^{\nu/3}$ curves do not show any crossing for $T > 1.2$. Since the transition is MF-like in this case, the behavior of ξ is clearly caused by large FSE. Numerical estimates of T_c obtained with the two methods are reported in Table I and look compatible. It is clear that for large ρ our method works better. As ρ is decreased, this new estimate becomes poorer, because the scaling exponent $\rho - 1$ [cf. Eq. (8)] is too small to yield a robust extrapolation of $A(L, T)$.

Discussion of experimental results.—A possible objection to the presence of the SG transition (supported by our results) is that in experiments on Ising-like SG no dAT line was detected. Here we consider, in particular, the most recent experiments on $Fe_{0.55}Mn_{0.45}TiO_3$ [4], where the ac susceptibilities were accurately measured in the presence of an external magnetic field. In order to relate external fields in our model to those used in experiments we look at how much the zero-field-cooled (ZFC) susceptibility at $T_c(h = 0)$, χ^*, decreases as h is increased. In Fig. 4 we plot $T_c(h)/T_c(0)$ vs $\chi^*(h)/\chi^*(0)$ in our model for $\rho = 1.5$. In experiments on $Fe_{0.55}Mn_{0.45}TiO_3$ [4] with fields of

TABLE I. Estimates of T_c: column 4 from Eqs. (6) and (7) and column 5 from the extrapolation of $A(L, T)$ by Eq. (8).

	ρ	h	T_c from $\chi_{\rm sg}$	T_c from $A(L, T)$
	1.2	0.0	2.24(1)	2.34(3)
	1.2	0.1	2.02(2)	1.9(2)
MF	1.2	0.2	1.67(3)	1.4(2)
	1.2	0.3	1.46(3)	1.5(4)
	1.25	0.0	2.191(5)	2.23(2)
	1.4	0.0	1.954(3)	1.970(2)
	1.4	0.1	∼1.5	1.67(7)
IRD	1.4	0.2	∼1.1	1.2(2)
	1.5	0.0	1.758(4)	1.770(5)
	1.5	0.1	—	1.46(3)
	1.5	0.15	—	1.20(7)
	1.5	0.2	—	0.8(2)

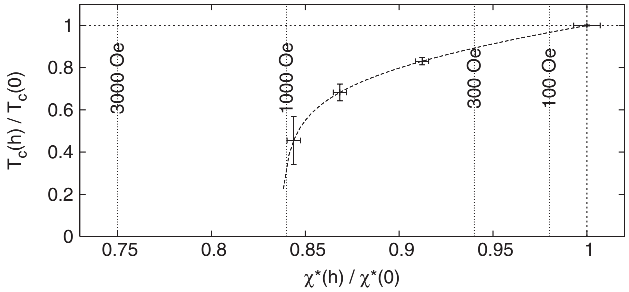

FIG. 4. Relative decrease of the critical temperature with increasing field ($\rho = 1.5$, $h = 0$, 0.1, 0.15, 0.2) versus relative decrease of χ^*, the ZFC susceptibility at $T_c(h = 0)$. The dashed curve is a guide for the eye.

magnitude 100 Oe, 300 Oe, 1000 Oe and 3000 Oe one has, respectively, $\chi^*(h)/\chi^*(0) = 0.98$, 0.94, 0.84, 0.75. These ratios, cf. Fig. 4, suggest that a SG transition is unlikely to be experimentally observed above $h = 1000$ Oe.

Increasing ρ, and/or considering $\bar{J}_{ij} \neq 0$, the critical field decreases. The $\rho = 1.5$ model considered above is approximately equivalent to a short-range system in $D = 4$. Therefore, in order to detect, or rule out, a SG phase in $D = 3$, it becomes even more important to work at small fields. The observation that the fields used in experiments on Ising-like materials are maybe too large to see a SG phase is in agreement with the results of Petit *et al.*, who studied both Ising-like and Heisenberg-like SG samples [2].

Conclusions.—By using a new method of data analysis, we have been able to identify a dAT line in the diluted power-law decaying interaction Ising SG chain at all values of the power analyzed, including values corresponding to short-range SG models below the UCD. The behavior below the dAT line may change with the dimension. We are presently studying this possibility.

These dAT lines were not found in the study of the fully connected version performed in Ref. [25], nor in Ref. [24] where a similar diluted model was simulated. There, T_c was estimated by using the scaling properties of ξ/L. As we have shown, this quantity suffers of strong FSE. We put forward an alternative method to discriminate between a pure paramagnetic phase at all temperatures and a finite temperature SG transition. An advantage of this method is that it mainly uses data at $T > T_c$.

For what concerns three dimensional real systems, we hint that the magnitude of the external fields used in experiments up to now might be too large to firmly rule out the presence of a dAT transition line. We suggest a range of fields ($h < 1000$ Oe) where the transition should take place in $Fe_{0.55}Mn_{0.45}TiO_3$ and we hope this may stimulate further experimental investigations, as in , e.g., the very recent study of Ref. [26].

This work has been partially supported by MEC, Contracts No. FIS2006-08533-C03 and No. FIS2007-60977. Part of the simulations were performed in the BIFI cluster.

[1] J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978).
[2] D. Petit, L. Fruchter, and I. A. Campbell, Phys. Rev. Lett. **83**, 5130 (1999); **88**, 207206 (2002).
[3] M. Gabay and G. Toulouse, Phys. Rev. Lett. **47**, 201 (1981).
[4] P. E. Jönsson *et al.*, Phys. Rev. B **71**, 180412(R) (2005); P. E. Jönsson and H. Takayama, J. Phys. Soc. Jpn. **74**, 1131 (2005); P. E. Jönsson *et al.*, J. Magn. Magn. Mater. **310**, 1494 (2007).
[5] G. Parisi, J. Phys. A **13**, 1887 (1980).
[6] S. Boettcher, Phys. Rev. Lett. **95**, 197205 (2005); S. Franz, G. Parisi, and M. A. Virasoro, J. Phys. I (France) **4**, 1657 (1994).
[7] T. Temesvari, Phys. Rev. B **78**, 220401(R) (2008).
[8] D. S. Fisher and D. A. Huse, Phys. Rev. B **38**, 386 (1988).
[9] F. Krzakala and O. C. Martin, Phys. Rev. Lett. **85**, 3013 (2000).
[10] E. Marinari, C. Naitza, and F. Zuliani, J. Phys. A **31**, 6355 (1998).
[11] F. Krzakala *et al.*, Phys. Rev. Lett. **87**, 197204 (2001).
[12] A. P. Young and H. G. Katzgraber, Phys. Rev. Lett. **93**, 207203 (2004).
[13] M. Sasaki *et al.*, Phys. Rev. Lett. **99**, 137202 (2007).
[14] T. Jörg, H. G. Katzgraber, and F. Krzakala, Phys. Rev. Lett. **100**, 197202 (2008).
[15] L. Leuzzi *et al.*, Phys. Rev. Lett. **101**, 107203 (2008).
[16] The value $z = 6$ is a compromise: the computer time is proportional to z but the critical temperature approaches zero for small z (with drawbacks in its evaluation).
[17] The effect of a random local field is very similar to a uniform one [12,25,27] but with numerical advantages.
[18] G. Kotliar, P. W. Anderson, and D. L. Stein, Phys. Rev. B **27**, 602 (1983); L. Leuzzi, J. Phys. A **32**, 1417 (1999).
[19] M. Campanino *et al.*, Commun. Math. Phys. **108**, 241 (1987).
[20] Relationship $\rho = 1 + (2 - \eta(D))/D$ [24] is possibly a better approximation—though it relies on the knowledge of the η exponent in short-range systems. For our purposes, i.e., to determine the UCD, our relationship is enough.
[21] K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996).
[22] To save computing time we simulated two replicas and express four-point C as the linear combination of $\overline{\langle h_i h_j \sigma_i^{(1)} \sigma_j^{(2)} \rangle}$, $\overline{\langle h_i \sigma_i^{(1)} \sigma_i^{(2)} \sigma_j^{(2)} \rangle}$ and $\overline{\langle \sigma_i^{(1)} \sigma_j^{(1)} \sigma_i^{(2)} \sigma_j^{(2)} \rangle}$.
[23] S. Caracciolo *et al.*, Nucl. Phys. B **403**, 475 (1993).
[24] H. G. Katzgraber, D. Larson, and A. P. Young, Phys. Rev. Lett. **102**, 177205 (2009).
[25] H. G. Katzgraber and A. P. Young, Phys. Rev. B **72**, 184416 (2005).
[26] Y. Tabata *et al.*, arXiv:0908.1937v1.
[27] G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, Phys. Rev. B **57**, 13617 (1998).