

3D Spin Glass and 2D Ferromagnetic XY Model: a Comparison

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Abstract

We compare the probability distributions and Binder cumulants of the overlap in the 3D Ising spin glass with those of the magnetization in the ferromagnetic 2D XY model. We analyze similarities and differences. Evidence for the existence of a phase transition in the spin glass model is obtained thanks to the crossing of the Binder cumulant. We show that the behavior of the XY model is fully compatible with the Kosterlitz-Thouless scenario. Finite size effects have to be dealt with by using great care in order to discern among two very different physical pictures that can look very similar if analyzed without large attention.

1 Introduction

The issue of the existence of a phase transition in the three dimensional Ising spin glass has been a hard and difficult problem for more than two decades (see for example [1, 2] and references therein). Today there are clear numerical evidences favoring the existence of a low temperature broken phase [3, 4, 5, 2], but a deeper understanding of the underlying physics still lacks. It is clear, for example, that one is very close to the lower critical dimension (LCD), but understanding the details of the influence of such effect is highly non-trivial.

Determining for example the infinite volume limit of the Edward-Anderson order parameter [6] (q_{EA}) has been beyond reach till very recently, and the existence of the phase transition (both in 3 and 4 dimensions) has been established by exhibiting the crossing of the finite size Binder parameter. One was able to show (for the 3D case see [3, 4]) that curves of $g_L(T)$, $g_{L+1}(T)$ as a function of T would cross at $T_c^{(L)}$, but it was impossible to determine the non-trivial limit of $g_L(T)$ for $L \rightarrow \infty$ at $T < T_c$ (and in the same way it was impossible to determine the large volume limit of q_{EA}). Only in the most recent period off-equilibrium techniques [7] and equilibrium simulations based on parallel tempering [8] have allowed a statistically significant determination of the 4D infinite volume order parameter q_{EA} .

We start here by noticing that the behavior of the Binder parameter $g_L(q)$ in the 3D spin glass is very reminiscent of the one one finds in the 2D XY model (without quenched disorder), $g_L(m)$ (here m is the magnetization). Even for quite large lattices the curves for different lattice volumes are well split in the high T phase, but seem to merge better than cross at low T . Only on very large lattices one can exhibit a non-ambiguous (but always very small) crossing [3, 5]. The XY 2D model shows that the order parameter is zero in the thermodynamical limit only very slowly when increasing L .

The same kind of effect could be appearing in the 3D Edwards-Anderson spin glass, and in order to be sure one is dealing with a real phase transition with a non-zero order parameter one has to be very careful, and to show that is keeping under control possible contamination. That is why we have decided to run a comprehensive comparison of the order parameter distributions for the 3D Edwards-Anderson spin glass and for the 2D XY model. A detailed paper by Binder [9], containing a study of the distribution functions for the Ising model, can be considered a methodological prototype to this kind of analysis, and can be used as a nice introduction to the finite size scaling techniques and ideas used in this setting.

Let us start by reminding the reader about some main points concerning the definition of the lower critical dimension. The lower and the upper critical dimensions (d_l and d_u respectively) are important in qualifying a statistical system. d_u is the minimal dimension where mean field predictions hold (apart from logarithmic corrections), while the LCD, d_l , is the maximal dimension where the finite T phase transition disappears. A typical example is the usual Ising model, with $d_l = 1$ and $d_u = 4$ [10].

Since a ϕ^3 term appears in the effective Hamiltonian of spin glasses (see [6, 11] and references therein) one expects that the upper critical dimension is $d_u = 6$. One of the possible ways to determine the lower critical dimension is based on the determination of the critical exponent η . One starts from the two points correlation function at the critical

point, $T = T_c$, that for $|\vec{x} - \vec{y}| \rightarrow \infty$ behaves as

$$\langle \phi(\vec{x})\phi(\vec{y}) \rangle \simeq |\vec{x} - \vec{y}|^{-(d-2+\eta)} . \quad (1)$$

The LCD is defined by

$$d_l - 2 + \eta(d_l) = 0 , \quad (2)$$

i.e. by the fact that there is no power law decay of the two point correlation function at the ($T = 0$) critical point. A (replica-symmetric) ϵ -expansion computation [12] gives

$$\eta = -\frac{1}{3}\epsilon + 1.2593\epsilon^2 + 2.5367\epsilon^3 , \quad (3)$$

where $\epsilon \equiv (6 - d)$. At order ϵ one is getting the promising estimate $d_l = 3$, that collapses when including the higher order contributions, that do not allow any real solution for $d_l \leq 6$. It is clear that because of one of the many reasons that could give troubles (for example replica symmetric breaking and poor convergence of the ϵ -expansion) here the ϵ -expansion is not helping in determining the LCD.

Equation (2) allows an estimate of d_l based on numerical estimates of the η exponent. In four dimensions, with Gaussian couplings, one finds $\eta = -0.35 \pm 0.05$ [7], while in $3D$ $\eta = -0.40 \pm 0.05$ [5]. The variation of η with d is small, and it seems safe to estimate $d_l \simeq 2.5$. Even if this result is somehow peculiar (since in the field theoretical approach [11] one does not see any trace of propagators with non-integer powers) it is confirmed by a mean field based analysis [13] where one builds up an interface and looks at its behavior. This mean-field computation gives $d_l = 2.5$, in excellent agreement with the numerical estimate.

Numerical simulations in $3D$ [3, 5, 2] have now shown clearly that there is a finite T phase transition, i.e. that $d_l < 3$. The broken phase is mean field like, and understanding more details about it will be the goal of this paper. It is also well established that in $2D$ one finds a $T = 0$ phase transition (see [2] and references therein). Summarizing, from state of the art numerical simulations one can deduce that $2 \leq d_l < 3$.

Also the fact that $d_u = 6$ is well supported by numerical results [14, 15]. In $6d$ one determines with good accuracy mean field exponents ($\gamma = 1$, $\beta = 1$ and $z = 4$), with logarithmic corrections (that have been detected in the equilibrium simulations).

Here we will try to shed more light on the difficult numerical simulations of the $3D$ Edwards Anderson spin glass. The main problem is probably in the fact that the system is very close to its LCD. So the apparent merging of the Binder parameters in the low T region, that has only recently been disentangled to show a significant crossing [3, 5], is dramatically reminiscent of the one one can observe in the case of a Kosterlitz-Thouless transition. We will try here to learn more about the effects of an anomalous situation like the Kosterlitz Thouless (KT) one, by looking for example to the Binder cumulant and to the overlap probability distribution $P(q)$. To do this we will discuss in same detail the structure of the order parameter probability distribution in the $2D$ XY model without disorder. We will stress how similar to the $3D$ spin glass things are at a first level of analysis, and where the relevant differences can be found. It is also remarkable that the pure $2D$ XY model has a peculiar *aging* behavior [16]: aging is one of the crucial features of spin glass systems, and its qualification is of large importance.

In the next section we will define our models, the physical observable quantities, and we will give details about our numerical simulations. In section (3) we discuss our results, by following in parallel the 2D XY model without disorder and the 3D spin glass. In section (4) we draw our conclusions.

2 Models, Observables and Simulations

We have studied the two dimensional XY model on a squared lattice. The volume is denoted by $V = L^2$, the hamiltonian is

$$\mathcal{H} = - \sum_{\langle x,y \rangle} \cos(\phi_x - \phi_y) , \quad (4)$$

where $\langle x,y \rangle$ denotes a sum over nearest neighbor site pairs, ϕ is a continuous real variable, and periodic boundary conditions are imposed on the system. This model shows an *infinite order* phase transition (with $\beta_c \approx 1.11$) [17], the Kosterlitz-Thouless transition. In accordance with the Mermin-Wagner theorem [10] there cannot be non-zero order parameters: the magnetization in the thermodynamical limit is zero for all $T > 0$. The KT transition is characterized by a change in the behavior of the two point correlation function, which goes from the exponential decay of the high temperature phase to the algebraic decay of the low temperature phase. The whole low temperature phase ($\beta > \beta_c$) is critical (the correlation length is infinite).

To simulate this model we have used the Wolff single cluster algorithm [18]. The simulations have been run at five different values of β in the low temperature phase: $\beta = 1.3, 1.4, 1.5, 1.7, 2.0$. For each value of β we have used the lattice sizes $L = 8, 16, 32, 64, 128, 256$. For each value of (β, L) we have used 200,000 iterations of the single cluster algorithm, discarding the first half for thermalization. The total CPU time required has been approximately one month on a 100 MHz Pentium based computer.

We have measured the probability distributions of

$$m_1 \equiv \frac{1}{V} \left| \text{Re} \sum_x \exp(i\phi_x) \right| , \quad (5)$$

that we denote as $P_1(m_1)$. We call m_1^{max} the value of m_1 where $P_1(m_1)$ is maximum and takes the value $P_1^{\text{max}} \equiv \text{Max}[P_1(m_1)]$. We have looked in detail to the first and second moments of $P_1(m_1)$, $\langle m_1 \rangle$ and $\langle m_1^2 \rangle$. We have also computed the Binder cumulant of the $P_1(m_1)$ distribution:

$$B_1 = \frac{1}{2} \left(3 - \frac{\langle m_1^4 \rangle}{\langle m_1^2 \rangle^2} \right) . \quad (6)$$

At low T one can study the XY model by using the spin wave approximation, that neglects the role of vortices (since they are suppressed at low T). In the $T \rightarrow 0$ limit all the spins point in the same direction, and (θ) is uniformly distributed, so that

$$\langle m_1^p \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \cos^p \theta , \quad (7)$$

and the Binder cumulant at $T = 0$ has the value

$$B_1(T = 0) = \frac{3}{4} . \quad (8)$$

To determine the relevant scaling behavior we use the fact that, for the XY model, $\chi \simeq L^{2-\eta(T)}$ and $\langle m^2 \rangle \equiv \chi/L^2$, where in the spin wave approximation

$$\eta(T) = \frac{T}{2\pi} , \quad (9)$$

is the anomalous dimension of the field. Moreover, since $P_1(m_1)$ is a probability distribution, normalized to one, with non zero maximum value (m_1^{\max}) (at least for finite values of the lattice sizes) and with $\langle m_1^2 \rangle \simeq L^{-\eta} \rightarrow 0$ (at finite temperatures) we have that¹

$$P_1^{\max} m_1^{\max} \simeq 1, \quad (10)$$

independently of the lattice size, L . Since

$$m_1^{\max} \simeq \langle m_1 \rangle \simeq \langle m_1^2 \rangle^{1/2} ,$$

we conclude that

$$\begin{aligned} m_1^{\max} &\simeq L^{-\eta(T)/2} , \\ \langle m_1 \rangle &\simeq L^{-\eta(T)/2} , \\ \langle m_1^2 \rangle &\simeq L^{-\eta(T)} , \\ P_1^{\max} &\simeq L^{\eta(T)/2} . \end{aligned} \quad (11)$$

The other model we have studied is the three-dimensional Ising spin glass with quenched random couplings J distributed with a Gaussian law. The Hamiltonian is

$$\mathcal{H} \equiv - \sum_{\langle i,j \rangle} \sigma_i J_{i,j} \sigma_j , \quad (12)$$

where the spin are defined on a three-dimensional cubic lattice and $\langle i, j \rangle$ denotes a sum over nearest neighbor pairs.

As usual [2] we have simulated two real replicas (σ and τ) with the same quenched couplings, and we have measured the overlap

$$q(\sigma, \tau) \equiv \frac{1}{V} \sum_i \sigma_i \tau_i , \quad (13)$$

and its probability distribution

$$P(q) = \overline{\langle \delta(q - q(\sigma, \tau)) \rangle} \quad (14)$$

where, as usual, we denote the thermal average with $\langle (\dots) \rangle$, and the average over the disorder distribution with $\overline{(\dots)}$. The Binder cumulant of the probability distribution $P(q)$ is

¹In the rest of the paper the symbol $A \simeq B$ means $A = O(B)$.

$$g \equiv \frac{1}{2} \left[3 - \frac{\overline{\langle q^4 \rangle}}{\langle q^2 \rangle^2} \right]. \quad (15)$$

We have run $L = 4, 6, 8, 10, 12$ and 16 lattices with $2048, 2560, 512, 512, 2048$ and 500 samples respectively. We have used the supercomputer APE-100 [19].

For simulating the spin glass model we have used the simple tempering method for small lattices ($L \leq 10$), and the parallel tempering scheme for large lattices ($L \geq 12$) (see [20, 21, 2] and references therein). Thanks to that we have kept under control the level of thermalization reached by the system, that is in all cases very good (for a discussion of the standard criteria of control see [21]). We have checked that the equalities established numerically in [4], and proven by Guerra [22] hold for our results, and that the $P(q)$ is well symmetric, supporting the reach of full thermalization.

3 Results

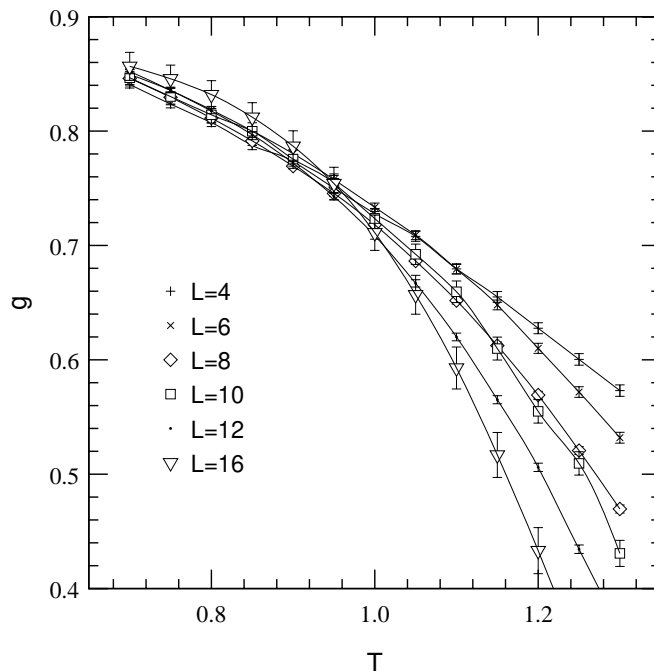


Figure 1: Binder cumulant for the 3D Ising spin glass. On the right, from top to bottom, curves and data points are for $L = 4, 6, 8, 10, 12$ and 16 .

In figures (1) and (2) we show the Binder cumulant and the probability distribution of the 3D Ising spin glass.

Let us discuss first the Binder cumulant. In figure (1) there are two different regions. In a high temperature region curves corresponding to different lattice sizes are clearly split (they tend to zero in the thermodynamical limit). At small temperature (i.e. for β larger

than $\beta_c^{\text{SG}} \approx 1.0$), on small lattice sizes (up to $L = 10$) curves coalesce, within our small error bars, in one. It is interesting to notice that defining a Binder cumulant based on three different replicas [23] allows a somehow easier determination of the critical behavior.

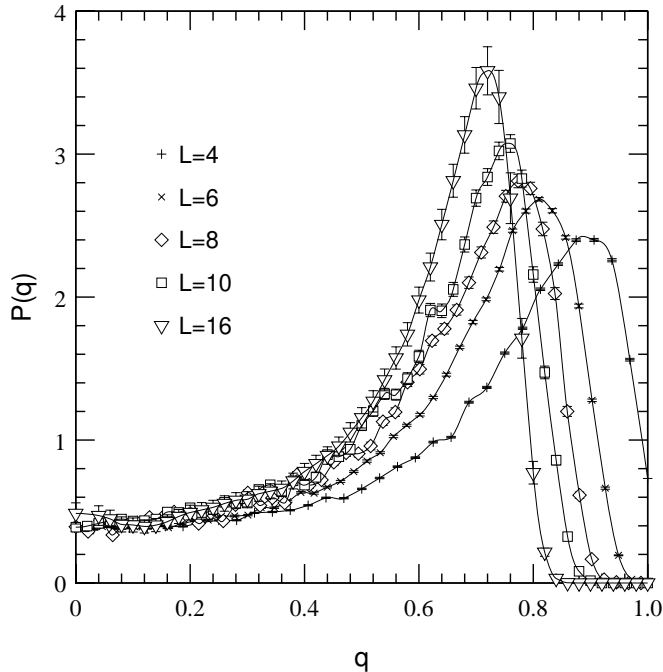


Figure 2: Probability distribution of the overlap, $P(q)$, for the 3D Ising spin glass. $T = 0.7$. From right to left curves and data points are for $L = 4, 6, 8, 10$ and 16.

Only when thermalizing a $L = 16$ lattice (quite large for current standards, and impossible to thermalize deep in the critical region without the use of parallel tempering [2]) one is able to exhibit a clear crossing between, for example, the $L = 8$ curve and the $L = 16$ curve. This implies the existence of a phase transition at finite temperature with a non-zero order parameter, $q_{\text{EA}} \neq 0$ (see Kawashima and Young [3] for the model with quenched binary couplings, $J = \pm 1$).

We can compare figure (1) with figure (3), where we show our numerical results for the Binder cumulant, B_1 , for the 2D XY model. Up to $L = 10$ the XY model and the 3D Ising spin glass have a very similar behavior: again, within error bars, in the low temperature region all the curves for different lattice sizes collapse in a single curve, without any visible sign of finite size effects.

The behavior of the full probability distribution of the order parameter (m_1 for the 2D XY model and q for the 3D Ising spin glass) is very similar. Figures (4) and (5), where we show $P_1(m_1)$ at $\beta = 1.3$ and $\beta = 2.0$ respectively, can be compared to the analogous figure for the spin glass $P(q)$, (2). The overall shapes are very similar. The peak shifts to the left, and in both cases $P(0)$ looks constant in our statistical precision.

We give in table (1), at $\beta = 1.3$, the expectation values of the observables shown figures (4) and (5). By fitting these values by using a single power fit we find

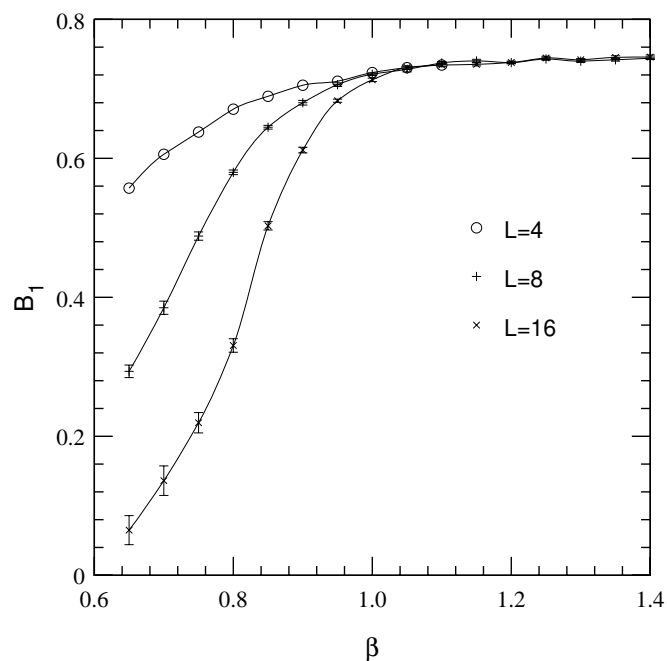


Figure 3: Binder cumulant, B_1 , for the 2D XY model. From top to bottom, $L = 4, 8$ and 16.

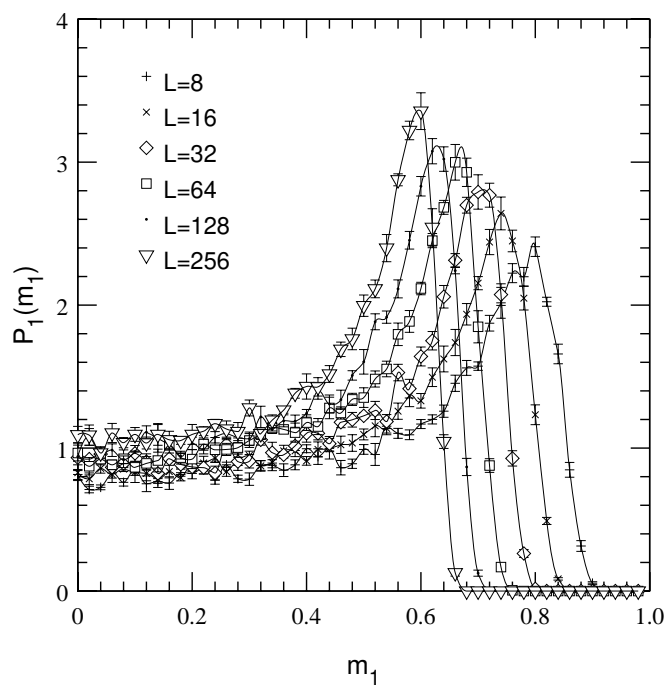


Figure 4: Probability distribution for the 2D XY model, $P_1(m_1)$, at $\beta = 1.3$.

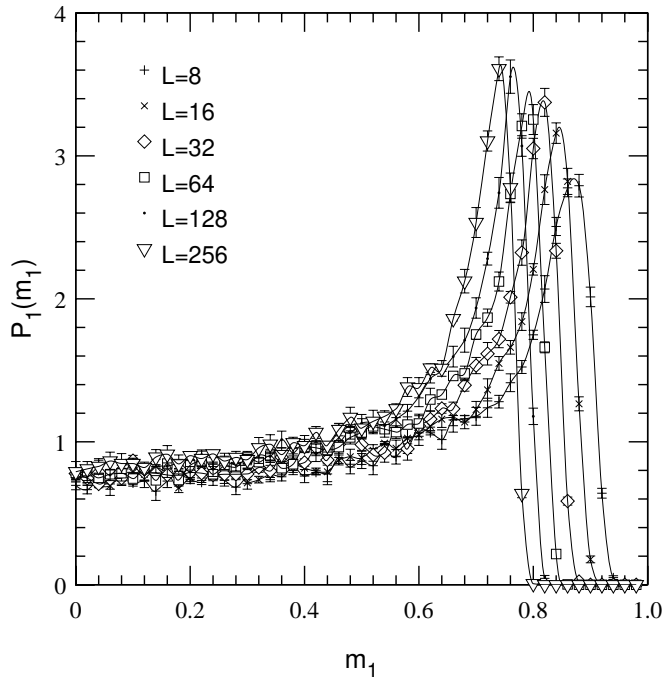


Figure 5: Probability distribution for the 2D XY model, $P_1(m_1)$, at $\beta = 2.0$.

$$\begin{aligned}
 m_1^{\max} &\simeq L^{-(0.08 \pm 0.01)}, \\
 \langle m_1 \rangle &\simeq L^{-(0.09 \pm 0.01)}, \\
 \langle m_1^2 \rangle &\simeq L^{-(0.17 \pm 0.01)}, \\
 P_1^{\max} &\simeq L^{+(0.09 \pm 0.01)}.
 \end{aligned} \tag{16}$$

These results are in remarkable agreement among them and in good agreement with the spin wave exact value $\eta(\beta = 1.3) = 0.12$. Corrections due to vortices are equivalent to a higher effective temperature [24], that undergoes here a 30% shift.

We have also established that a power fit to a non-zero infinite volume order parameter of the form

$$m_1^{\max}(L) = m_1^{\max}(\infty) + \frac{A}{L^B}, \tag{17}$$

with $m_1^{\max}(\infty)$ different from zero and A and B constant is excluded by the data.

Figures (4) and (5) are interesting: they show a finite size non-trivial behavior that we know, from theoretical ideas (the Mermin-Wagner theorem), and from the analysis of the numerical data, will converge to a zero centered delta function limiting probability distribution in the infinite volume limit. This is the point we want to stress. Since the 3D spin glass has a very similar behavior (and even for the 4d model, where the crossing of the Binder cumulant is clear, it is non-trivial to show that q_{EA} tends to a non-zero limit) it is crucial to understand where differences are.

We also want to stress that $P_1(m_1)$ shows a clear plateau, roughly L -independent, close to the $m_1 \simeq 0$ region. The plateau height grows with the lattice size (in a statistically significant way in our numerical data, see (1)). This is one of the interesting results of this note: the infinite volume $2D$ XY m_1 delta function is constructed from the increasing finite volumes by a finite m_1 peak that shifts towards $m_1 \simeq 0$, and by a plateau in the $m_1 \simeq 0$ region that slowly increases with the lattice size, to eventually match the peak in the $m_1 = 0$ delta function.

We have repeated this analysis for the overlap probability distribution $P(q)$ of the $3D$ spin glass (see figure (2)). The best scaling fit of the peak position, q_M , where the probability distribution is maximum, by a power law (the data are in table (2)) gives

$$q_M = (0.70 \pm 0.02) + (1.6 \pm 0.7)L^{-(1.5 \pm 0.4)}, \quad (18)$$

where $T = 0.7$. In this fit we have used all lattice volumes ($L \leq 16$). The fit had a $\chi^2/\text{dof} = 0.15$. This thermodynamical value we get for q_{EA} is close to the value that has been extracted from an off-equilibrium simulation ($q \simeq 0.7$) [5]. The best (two parameter) fit obtained by fixing $q_M = 0.7$ (considered as an input from the dynamical simulations) gives compatible results with smaller errors. In figure (6) we show the q_M data versus $L^{-1.5}$ (see also table (2)), and the curve from the best (two parameter) fit.

From the numerical data for the $3D$ spin glass (that are from a state of the art large scale numerical simulation) we cannot exclude the possibility of $q_{EA} = 0$ in the infinite volume limit. We find that the best fit (that uses in this case only $L \geq 6$ data)

$$q_M = (1.0 \pm 0.1)L^{-(0.12 \pm 0.02)} \quad (19)$$

is very good. So, even if the scenario of a non-zero overlap is favored (the static value is equal to the dynamic one, the exponent of a decay to $q = 0$ is very small) in the $3D$ case we cannot use this limit to be sure of the existence of a phase transition with a non-zero order parameter (in $4d$ recent high statistics data allow to establish this evidence [8]). The safe evidence for the existence of a phase transition in the $3D$ spin glass relies in this moment on the statistically significant crossing of the finite L Binder cumulant [3, 5], that makes visible fine details of the equilibrium probability distribution.

Also the behavior of $P(0)$ turns out to be the potential source of many ambiguities. We have seen that in the XY model it grows very slowly with the lattice size, in order to asymptotically contribute to the $m_1 = 0$ delta function. Also in the $3D$ spin glass, where in a mean-field like broken phase we expect a finite limit for $P(0)$ we observe a constant plateau with a (non necessarily statistically significant) growth for $L = 16$. This behavior contributes to falsify the droplet model picture, where one would expect $P(0)$ to decrease with the lattice size.

4 Conclusions

We have shown that the two dimensional ferromagnetic XY model and the three dimensional Ising spin glass finite volume order parameter probability distributions behave very similarly. The Binder cumulants on small lattice volumes show a similar *merging* at low T . Only on large lattices the $3D$ spin glass exhibits a crossing typical of a phase transition.

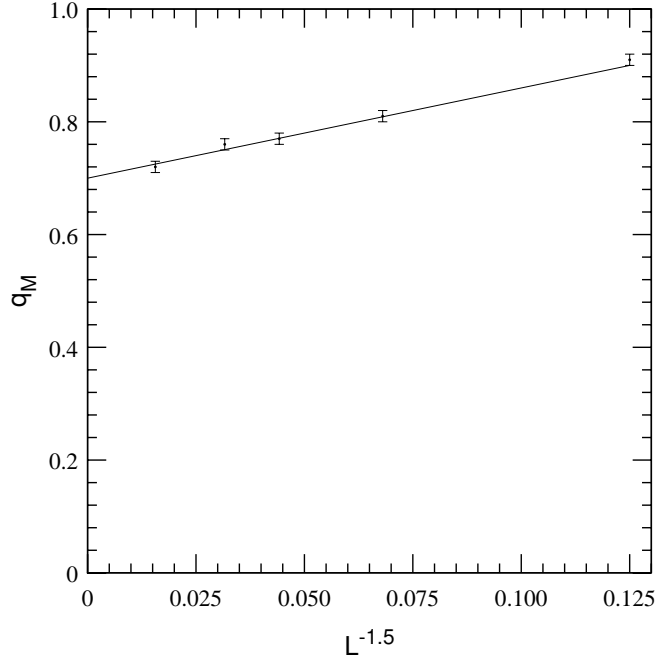


Figure 6: Value of the overlap q_M such that $P(q)$ is maximum (3D Ising spin glass). The continuous line is the fit described in the text. $T = 0.7$.

L	m_1^{\max}	$\langle m_1 \rangle$	$\langle m_1^2 \rangle$	P_1^{\max}	$P_1(0)$
16	0.74(1)	0.485(6)	0.283(4)	2.64(9)	0.83(5)
32	0.70(1)	0.456(5)	0.260(3)	2.79(8)	0.93(2)
64	0.66(1)	0.431(5)	0.231(3)	3.00(9)	0.97(6)
128	0.62(1)	0.405(4)	0.205(2)	3.08(7)	0.94(9)
256	0.60(1)	0.382(5)	0.183(3)	3.36(11)	1.09(6)

Table 1: Numerical data for the 2D XY model, $\beta = 1.3$. See the text for more details.

L	q_M	$P(0)$
4	0.91(1)	0.398(3)
6	0.81(1)	0.376(5)
8	0.77(1)	0.39(2)
10	0.76(1)	0.39(2)
16	0.72(1)	0.49(7)

Table 2: Numerical data for the 3D Ising spin glass, $T = 0.7$. See the text for more details.

The results that we have discussed for the XY model are completely compatible with the KT predictions. We have analyzed the finite volume behavior of the peak of the finite volume order parameter probability distribution. In the case of the XY model the preferred limit is zero. In the spin glass case the preferred value is non-zero, and compatible with an off-equilibrium estimate, but from the present data one cannot rule out the possibility of the position of the peak going to zero in the infinite volume limit.

We have also established that $P(0)$ in the KT scenario has a finite volume non-zero value, that increases in the infinite volume limit. In finite volume one can then exhibit probability distributions with the same shape of that of a finite dimensional spin glass that have a trivial thermodynamic limit (a delta function in the origin). Analyzing finite size effects is crucial before reaching conclusions about the critical behavior. In the $3D$ spin glass good evidence for the existence of a mean field like phase transition is based on a dynamical determination of the Edward-Anderson order parameter and on the crossing of the Binder cumulant on large lattices, but determining with good precision the shape of $P(q)$ on large lattice sizes will be important for making more details of the critical behavior crystal clear.

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