

Numerical study of the Sherrington-Kirkpatrick model in a magnetic field

Alain Billoire and Barbara Coluzzi

Service de Physique Théorique, CEA-Saclay, Orme des Merisiers, 91191 Gif-sur-Yvette, France

(Received 7 February 2003; published 29 August 2003)

We study numerically the Sherrington-Kirkpatrick model as a function of the magnetic field h , with fixed temperature $T=0.6T_c$. We investigate the finite size scaling behavior of several quantities, such as the spin-glass susceptibility, searching for numerical evidences of the transition on the de Almeida-Thouless line. We find strong corrections to scaling which make difficult to locate the transition point. This shows, in a simple case, the extreme difficulties of spin-glass simulations in a nonzero magnetic field. Next, we study various sum rules (consequences of stochastic stability) involving overlaps between three and four replicas, which appear to be numerically well satisfied, and in a nontrivial way. Finally, we present data on $P(q)$ for a large lattice size ($N=3200$) at low temperature $T=0.4T_c$, where the shape predicted by the replica symmetry breaking solution of the model for a nonzero magnetic field is visible.

DOI: 10.1103/PhysRevE.68.026131

PACS number(s): 64.60.-i, 05.10.Ln

I. INTRODUCTION

The Sherrington-Kirkpatrick (SK) model was introduced some time ago [1] as a mean-field model for spin glasses. Its analytical, replica symmetry breaking (RSB), solution [2] displays, in the glassy phase, intriguing features such as an infinite number of pure states, described by an order parameter which is the nontrivial probability distribution of the overlap between two of them, $P(q)$.

The applicability of the mean-field picture to short range spin glasses [3] is however still debated, and an alternative (family of) scenario(s) called the droplet model has been put forward by several authors. One may, in principle, distinguish between these two theories of finite-dimensional spin glasses by observing the fate of the glassy phase for a nonzero magnetic field. In the SK model (and accordingly in the mean field picture) one finds [4,5] that a magnetic field (of absolute value) lower than the critical de Almeida-Thouless (AT) value $h_{AT}(T)$ [6] does not destroy the spin-glass ordering, since the number of states is still infinite. On the other hand, in the droplet picture one has only two states at $h=0$, related by the global inversion symmetry of the spins, and any small magnetic field makes the system paramagnetic [7–9].

It turned out unfortunately [10–24] that strong finite size corrections make it difficult to obtain a clear answer from equilibrium simulations in a magnetic field (of the system sizes that can presently be handled). Very recently, for example, the authors of a study of the local excitations of the Edwards-Anderson (EA) model [23] claim that there is no transition, whereas results on the out-of-equilibrium behavior of this model [24] appear in good agreement with the mean-field picture. On the theoretical side, it has been recently proposed [25] that the transition below the upper critical dimension $d_u=8$ is governed by a fixed point different from the AT mean-field fixed point.

This state of affairs motivated us to revisit the case of the SK model in a magnetic field. There have been indeed few numerical studies on the SK model in a fixed magnetic field h [15,16,26–29], and the behavior of the system as a function of the magnetic field at fixed T has never been numeri-

cally investigated to our knowledge.

We present results on the spin-glass susceptibility and different dimensionless ratios of $P(q)$ moments, looking for the quantities that are most appropriate for obtaining numerical evidence of the transition on the AT line. We will show in particular that finite size effects are strongly reduced if one considers the probability distribution of the absolute value of the overlap, and not the overlap itself.

We moreover consider the overlaps between three and four replicas, checking the validity of some relations (the so called stochastic stability sum rules) which are an evident manifestation of the non-self-averageness of $P(q)$ [30,31] that have been recently derived under very general properties [32–35].

Finally, we present data for $P(q)$ in a magnetic field, where the shape predicted by the solution of the model, with two peaks separated by a continuum is visible. All simulations presented up to now show only a broad peak around q_{EA} . Both large system sizes (we have $N=3200$) and low temperature (we go down to $T=0.4$) are needed to see this asymptotic shape.

II. MODEL AND OBSERVABLES

The Sherrington-Kirkpatrick spin-glass model with N sites [4,5] is described by the Hamiltonian

$$\mathcal{H}_J = \sum_{1 \leq i < j \leq N} J_{ij} \sigma_i \sigma_j - h \sum_{1 \leq i \leq N} \sigma_i, \quad (1)$$

where $\sigma_i = \pm 1$ are Ising spins. The sum runs over all spin pairs and J_{ij} are quenched identically distributed independent random variables with mean value $J_{ij} = 0$ and variance $1/N$. We take $J_{ij} = \pm N^{-1/2}$.

In order to sample the probability distribution of the overlap $P(q)$, one usually considers two independent replicas $\{\sigma_i\}$ and $\{\tau_i\}$ evolving contemporaneously and independently:

$$Q = \frac{1}{N} \sum_{i=1}^N \sigma_i \tau_i, \quad (2)$$

$$P(q) \equiv \overline{P_J(q)} \equiv \overline{\langle \delta(q - Q) \rangle}, \quad (3)$$

where the thermal average $\langle \dots \rangle$ corresponds to the time average during the simulation, whereas $\overline{(\dots)}$ stands for the average over the J_{ij} realizations. This is the order parameter of the model, which in the thermodynamic limit behaves like

$$P(q) = \begin{cases} \delta(q - q_{EA}), & |h| > h_{AT}(T) \\ x_m \delta(q - q_m) + \tilde{P}(q) + x_M \delta(q - q_{EA}), & 0 < |h| < h_{AT}(T) \\ \frac{1}{2} [\tilde{P}(q) + \tilde{P}(-q)] + \frac{x_M}{2} [\delta(q - q_{EA}) + \delta(q + q_{EA})], & h = 0, T < T_c, \end{cases} \quad (4)$$

where $h_{AT}(T)$ is the critical value of the magnetic field on the AT line, with $h_{AT}(T) \sim (4/3)^{1/2} (T_c - T)^{3/2}$ for $T \rightarrow T_c^-$ ($T_c = 1$ in this model) [6]. For $T \rightarrow T_c^-$ one finds that $x_m \propto q_m \propto h^{2/3}$, and $(q_{EA} - q_m) \propto (x_M - x_m) \propto [h_{AT}(T) - h]$. Note that at $h = 0$ the function $P(q)$ is symmetric, reflecting the global flip $\{\sigma_i\} \rightarrow \{-\sigma_i\}$ symmetry of the system, and the δ function at q_m disappears. As we will discuss in detail, this implies a singular behavior for different quantities in the $h \rightarrow 0$ limit, which is among the main sources of difficulties in finding evidence for the phase transition in a magnetic field.

In order to locate numerically phase transitions, in our case the AT line, it is a common practice to consider dimensionless ratios of moments of $P(q)$, which are expected to have a fixed point (with respect to N) at the critical point, such as the (connected) Binder parameter [36,37]

$$B(h, T) = \frac{1}{2} \left(3 - \frac{\overline{\langle (q - \langle q \rangle)^4 \rangle}}{\overline{\langle (q - \langle q \rangle)^2 \rangle}^2} \right) \quad (5)$$

and the skewness

$$S(h, T) = \frac{\overline{\langle (q - \langle q \rangle)^3 \rangle}}{\overline{\langle (q - \langle q \rangle)^2 \rangle}^{3/2}}. \quad (6)$$

Here, $B(h, T)$ is defined in such a way that it is 0 for a Gaussian distribution and 1 for a two-equal-weight δ -function distribution, whereas the skewness is a measure of $P(q)$ asymmetry, which is nonzero in our case of nonzero magnetic field.

Further evidence for the presence of a phase transition should come from the behavior of the spin-glass (SG) susceptibility

$$\chi_{SG}(h, N) \propto N(\overline{\langle q^2 \rangle} - \overline{\langle q \rangle}^2), \quad (7)$$

which is expected to diverge, in the thermodynamic limit, when entering in the spin-glass phase, like

$$\chi_{SG}(h, \infty) \propto \frac{1}{h - h_{AT}^+}, \quad h \rightarrow h_{AT}^+, \quad T \text{ fixed.} \quad (8)$$

According to usual finite size scaling arguments, the finite size behavior is (for h near to h_{AT})

$$\chi_{SG}(h, N) = N^{1/3} \tilde{\chi}_{SG}[N^{1/3}(h - h_{AT})], \quad T \text{ fixed.} \quad (9)$$

The finite size behavior of the spin-glass susceptibility in the SK model on the AT line was numerically studied in Ref. [15], and the scaling $\approx N^{1/3}$ was checked.

The non-self-averageness of $P(q)$ is among the many fascinating features of the SK model. For instance, considering four replicas of the system, one finds [31] that $\overline{P_J(q_{12})P_J(q_{34})} \neq \overline{P(q_{12})P(q_{34})}$, whereas the following relations hold:

$$\begin{aligned} \overline{P(q_{12}, q_{34})} &\equiv \overline{P_J(q_{12})P_J(q_{34})} \\ &= \frac{2}{3} \overline{P(q_{12})P(q_{34})} + \frac{1}{3} \overline{P(q_{12})\delta(q_{12} - q_{34})}, \end{aligned} \quad (10)$$

$$\begin{aligned} \overline{P(q_{12}, q_{13})} &\equiv \overline{P_J(q_{12})P_J(q_{13})} \\ &= \frac{1}{2} \overline{P(q_{12})P(q_{13})} + \frac{1}{2} \overline{P(q_{12})\delta(q_{12} - q_{13})}. \end{aligned} \quad (11)$$

These kind of relations, which are nontrivially verified if the replica symmetry is broken [$P(q) \neq \delta(q - q_{EA})$], were recently derived under very general conditions [32–35], such as stochastic stability [38]. Infinitely many sum rules follow. We consider in particular the following relations:

$$R_{1234}^a(h, T) = \overline{\langle q_{12}q_{34} \rangle} - \frac{2}{3} \overline{\langle q \rangle}^2 - \frac{1}{3} \overline{\langle q^2 \rangle} = 0, \quad (12)$$

$$R_{1234}^b(h, T) = \frac{\overline{\langle q_{12}q_{34} \rangle} - \overline{\langle q \rangle}^2}{\overline{\langle q^2 \rangle} - \overline{\langle q \rangle}^2} = \frac{\chi_{SG}^{1234}(h, T)}{\chi_{SG}(h, T)} = \frac{1}{3}, \quad (13)$$

$$R_{1213}^a(h, T) = \overline{\langle q_{12}q_{13} \rangle} - \frac{1}{2} \overline{\langle q \rangle}^2 - \frac{1}{2} \overline{\langle q^2 \rangle} = 0, \quad (14)$$

$$R_{1213}^b(h, T) = \frac{\overline{\langle q_{12}q_{13} \rangle} - \overline{\langle q \rangle}^2}{\overline{\langle q^2 \rangle} - \overline{\langle q \rangle}^2} = \frac{\chi_{SG}^{1213}(h, T)}{\chi_{SG}(h, T)} = \frac{1}{2}, \quad (15)$$

$$R_{1234}^2(h, T) = \overline{\langle q_{12}^2 q_{34}^2 \rangle} - \frac{2}{3} \overline{\langle q^2 \rangle}^2 - \frac{1}{3} \overline{\langle q^4 \rangle} = 0, \quad (16)$$

$$R_{1213}^2(h, T) = \overline{\langle q_{12}^2 q_{13}^2 \rangle} - \frac{1}{2} \overline{\langle q^2 \rangle}^2 - \frac{1}{2} \overline{\langle q^4 \rangle} = 0. \quad (17)$$

Relations $R_{1234}^{a,b}(h,T)$ and $R_{1213}^{a,b}(h,T)$, which have to our knowledge never been previously investigated numerically, are expected to be verified only at nonzero magnetic field, since these relations are not invariant under a global flip, and an infinitesimal magnetic field was implicit in the derivation of Eqs. (10) and (11). On the other hand, relations $R_{1234}^2(h,T)$ and $R_{1213}^2(h,T)$ are valid for a zero magnetic field also, and were already studied (for three-dimensional (3D) and 4D Ising spin glasses at zero magnetic field [3,39,40]).

We also measured the following ratios of moments which are nonzero when the system is non-self-averaging, and have been introduced for locating the transition point [28,29]:

$$G(h,T) = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\langle q^4 \rangle - \langle q^2 \rangle^2}, \quad (18)$$

$$G_c(h,T) = \frac{\overline{\langle (q - \langle q \rangle)^2 \rangle^2} - \overline{\langle (q - \langle q \rangle)^2 \rangle}^2}{\langle (q - \langle q \rangle)^4 \rangle - \langle (q - \langle q \rangle)^2 \rangle^2}, \quad (19)$$

$$A(h,T) = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\langle q^2 \rangle^2}, \quad (20)$$

$$A_c(h,T) = \frac{\overline{\langle (q - \langle q \rangle)^2 \rangle^2} - \overline{\langle (q - \langle q \rangle)^2 \rangle}^2}{\langle (q - \langle q \rangle)^2 \rangle^2}. \quad (21)$$

In the infinite volume limit, $G(h,T)$ is expected to take the constant value 1/3 in the glassy phase because of relation (10), whereas $G_c(h,T)$, $A(h,T)$, and $A_c(h,T)$ are nontrivial functions of h and T , which are zero in the whole paramagnetic phase.

These parameters should be particularly useful when the Binder parameter behaves non monotonically, taking both positive and negative values, as it is found to happen when there is no time-reversal symmetry in the Hamiltonian [15,17,20,41,42] (such as in our case of nonzero magnetic field) and in systems where the mean-field solution is one-step replica symmetry breaking [43]. Their behavior has been extensively studied and they have been applied to a number of models [28,29,41,42,44,45].

The study of A and A_c allows us to check if the numerator in G and G_c is really nonzero or if it approaches zero for increasing volumes together with (or more slowly than) the denominator [28,29]. This is obviously not expected to happen in the glassy phase of the SK model. As a matter of fact, it was shown [29] that G and G_c should take the universal values 1/3 and 13/31, respectively, at zero temperature for any finite volume Ising system under quite general hypothesis, i.e., even if the order parameter is self-averaging.

The connected parameter G_c should be the most effective quantity to look at for locating the transition point, since it seems to be the one that is less affected by finite size corrections to scaling [29].

Relations R_{1234}^b , R_{1213}^b should behave as G and are in principle good candidates for obtaining evidence of the tran-

sition. Nevertheless, we will show that their finite size behavior, as well as the one of G itself, is definitely different from that of G_c (at least for the considered N values) and that they do not help in locating the transition point.

The main source of finite size effects is the global reversal of all spins. It does not occur in the thermodynamic limit, but when h is exactly zero. It does occur however in a finite volume, and as a consequence $P(q)$ develops a tail in the $q < 0$ region. This tail is significant [16,27] even for a size as large as $N = 1024$ and a magnetic field value $h = 0.3$ (at temperature $T = 0.6$). This was observed also in finite-dimensional systems [11,15,16,20] and it is expected to strongly affect the scaling of different quantities. In order to reduce its importance, one may use [14,15] the ‘‘absolute’’ spin-glass susceptibility defined as

$$\chi_{SG}^{abs}(h,N) = N(\overline{\langle q^2 \rangle} - \overline{\langle |q| \rangle}^2). \quad (22)$$

More generally, one can define ‘‘absolute’’ variants of all quantities defined in Eqs. (5), (6), and (12)–(21). In the following we will systematically study the differences between usual quantities and absolute ones (that will be labeled by the superscript *abs*), trying to clarify which are the most appropriate to look at in order to get evidence for the transition.

III. SIMULATIONS

We fixed the temperature at $T = 0.6$, where the AT line corresponds to the critical value $h_{AT}(T = 0.6) \approx 0.382$ [46]. We use the magnetic parallel tempering algorithm (h-PT), described in detail in our previous paper [27]. We consider $n = 49$ replicas, each one at a different magnetic field h from a set of n different values both within and without the AT lines, from $h_{min} = -0.6$ to $h_{max} = 0.6$ at equally spaced intervals of $\delta h = 0.025$. Exchange of h values between nearest neighbor replicas are allowed with the usual Monte Carlo acceptance probability. Moreover, the sign of all spins of a replica at $h = 0$ can be reversed with probability 1/2. This makes easier the passage from negative to positive h values and vice versa.

This h-PT algorithm is ideally suited to obtain the behavior of quantities as a function of the magnetic field at fixed temperature. However, it was found [27] that its efficiency rapidly decreases when simulating large systems, most probably because of chaos with the magnetic field. At variance with the case of temperature chaos, the effect of chaos with the magnetic field becomes evident already on a size of order $N = 1024$ and $\delta h \approx 0.15$. This means that the phase spaces explored by the system at equilibrium at h and $h + \delta h$ become quite different when $\delta h \approx 0.15$. Therefore, $N = 1024$ is the largest size we could thermalize with this method.

We perform 50 000 + 50 000, 100 000 + 100 000, and 300 000 + 300 000 h-PT sweeps for $N = 64$, 256, and 1024, respectively, the first half of each run being discarded from the statistics. Thermalization was checked by comparing the data obtained in the second part with the ones of the second quarter. We simulated four sets of replicas evolving contemporaneously and independently (i.e., $49 \times 4 = 196$ replicas). Data are averaged over 256 disorder configurations for each

system size. Statistical errors are evaluated from (disorder) sample-to-sample fluctuations by using the Jack-knife method.

Looking for evidences of the shape of $P(q)$ with $h \neq 0$ predicted by the solution of the model [Eqs. (4)], we performed a large scale simulation for a system of $N=3200$ spins, with the usual PT in temperature algorithm, taking $n=38$ equally spaced temperature values between $T_{min}=0.4$ and $T_{max}=1.325$, at magnetic field $h=0.3$. Results were averaged over 128 different disorder realization and we performed 400 000+400 000 PT steps for each sample, checking thermalization by comparing the $P(q)$ obtained in the second half and in the second quarter of the run.

IV. RESULTS AND DISCUSSION

A. Energy, magnetization, and magnetic susceptibility

We plot in Fig. 1 the energy density and the magnetization as a function of h for the different sizes considered. In the same figure, we also present data on the mean overlap $\overline{\langle q \rangle}$ and on the mean absolute value of the overlap $\overline{\langle |q| \rangle}$. It is evident from these data that the two quantities definitely differ for h as large as $h \approx 0.4$ (i.e., larger than h_{AT}) for $N=64$ and up to $h \approx 0.2$ for $N=1024$.

In Fig. 2 we plot the magnetic susceptibility computed as

$$\chi(h, N) = \frac{\partial \overline{\langle m \rangle}}{\partial h} \quad (23)$$

and as

$$\chi(h, N) = N\beta(\overline{\langle m^2 \rangle} - \overline{\langle m \rangle}^2). \quad (24)$$

An excellent agreement¹ is observed between the two estimates, showing that a good sampling has been achieved. We also plot the analytical estimate [47] (obtained in the so-called Parisi approximation for the Landau potential, and for $T \rightarrow T_c^-$)

$$\chi(h, \infty) = 1 - (3/4)^{2/3} h^{4/3}, \quad (25)$$

which is in quite good agreement with the data for h not too small.² In the thermodynamic limit, $\chi = \beta(1 - \overline{\langle q \rangle}) = \beta/\beta = 1$ in the whole spin-glass phase for $h \rightarrow 0$. On a finite system however, one must take into account the symmetry with respect to the flip of all the spins and $\chi(h=0, \infty) = \beta(1 - \overline{\langle q \rangle}) = \beta \approx 1.666$. Our data for χ show clearly the cross-over between these $h=0$ and $h \neq 0$ regimes. Figure 2 shows that finite size effects are positive for low h and negative for larger h . This change of sign must occur since the suscepti-

¹Although formulas (23) and (24) are identical mathematically, their Monte Carlo estimates can disagree, if the sampling is bad or if δh [we use finite difference to estimate Eq. (23)] is too large.

²A different formula appears in [48,49], with the order $h^{4/3}$ term multiplied by 7/3.

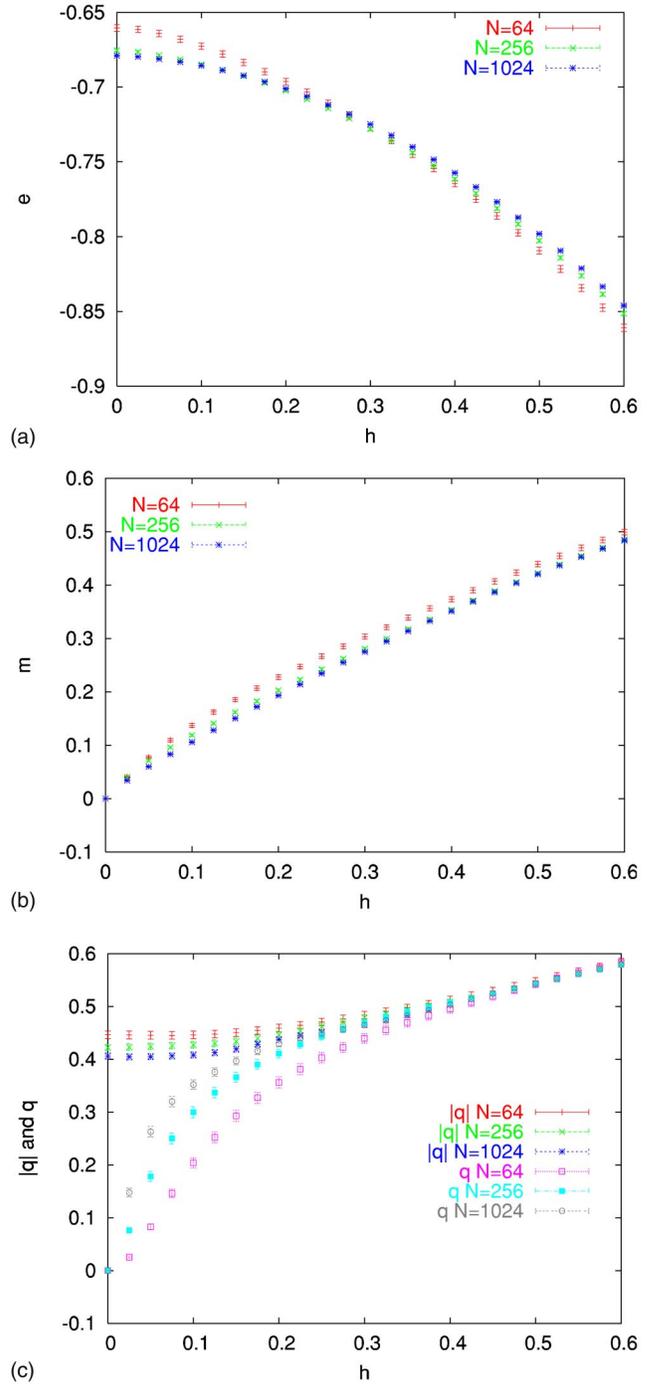


FIG. 1. (a) The energy density (b) the magnetization density, and (c) the mean value of the overlap: $\overline{\langle q \rangle}$ and $\overline{\langle |q| \rangle}$ at $T=0.6$, as a function of the magnetic field, for the different system sizes.

bility has sizable finite size corrections, whereas the magnetization is (trivially) size independent for $h=0$ and very weakly size dependent for large h .

For a better clarification of the situation, we also consider the absolute magnetic susceptibility χ^{abs} (see the same figure on the right), obtained from the probability distribution of the absolute value of the magnetization. Note that for the absolute susceptibility the estimates of Eqs. (23) and (24) do

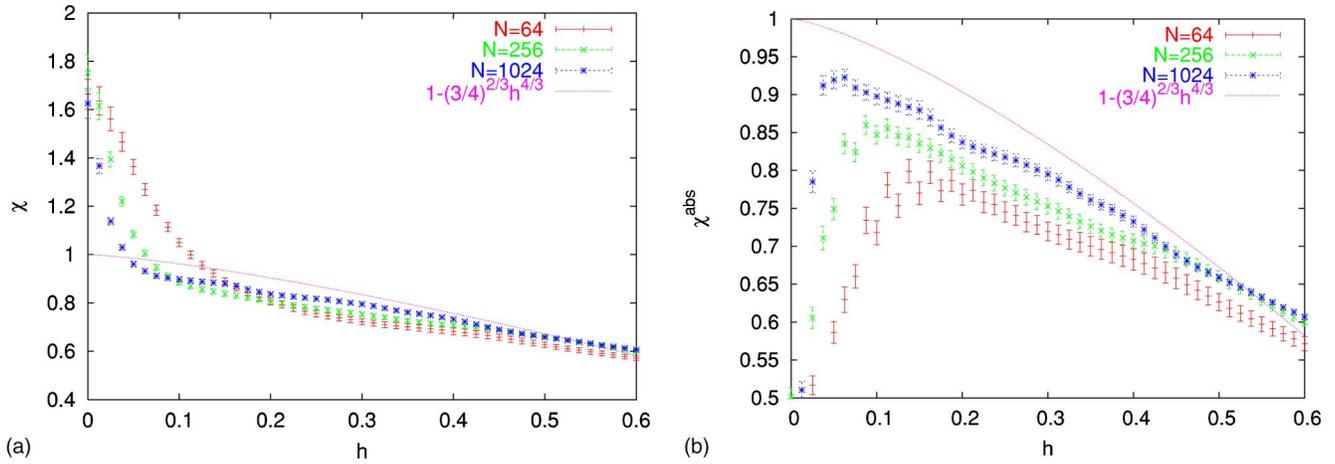


FIG. 2. (a) Usual magnetic susceptibility at $T=0.6$, as a function of the magnetic field, for the different values of the system size, compared with the predicted infinite volume analytic behavior (see text). (b) The magnetic susceptibility from the absolute value of the magnetization. In both plots the two estimates of the susceptibility, Eqs. (23) and (24), are plotted.

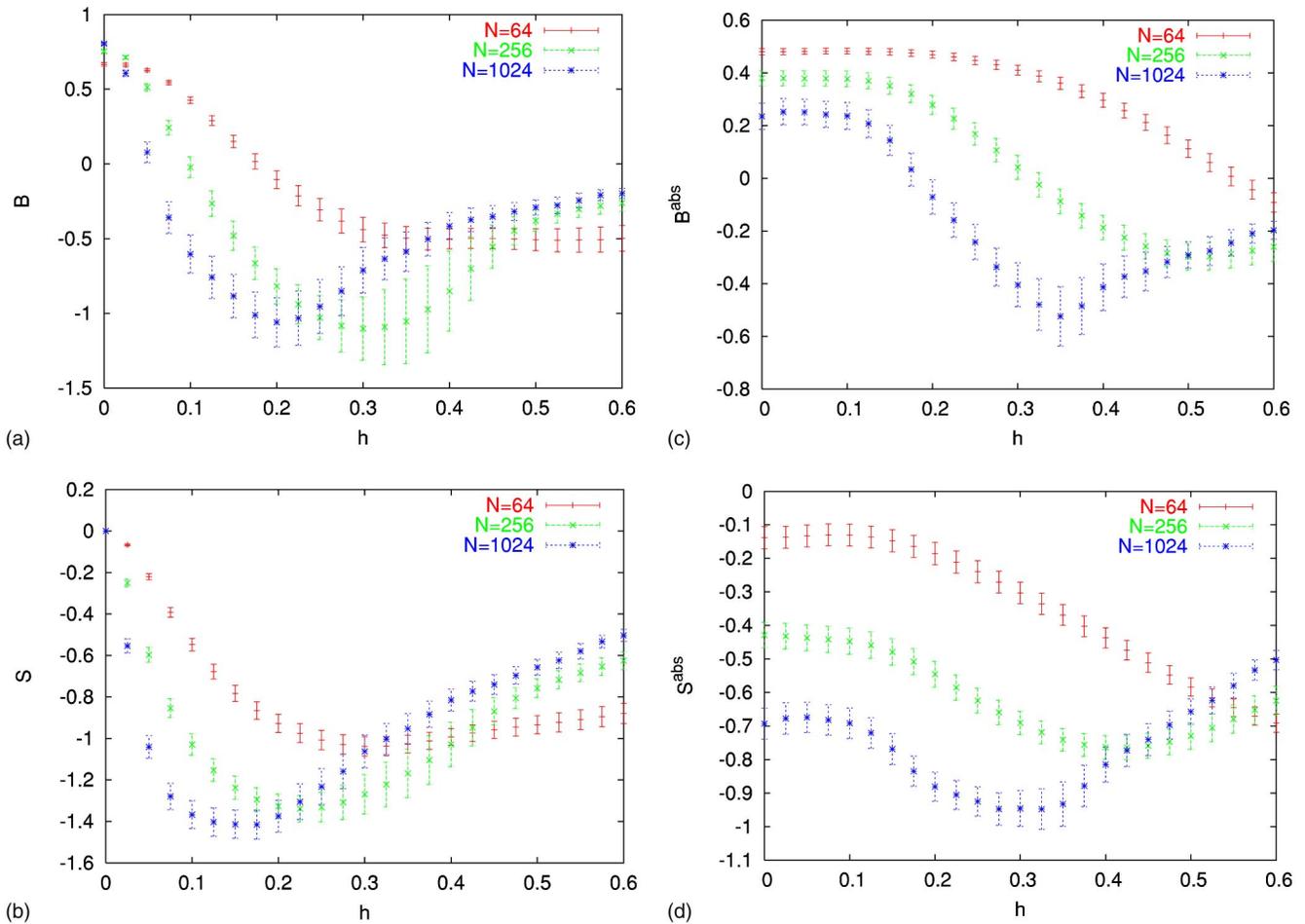


FIG. 3. The behavior of the Binder parameter $B(h, T)$ (a) and of the skewness $S(h, T)$ (b) at $T=0.6$, as a function of the magnetic field for the different system sizes. Here $h_{AT} \approx 0.382$. On the right are plotted the corresponding quantities $B^{abs}(h, T)$ (c) and $S^{abs}(h, T)$ (d), obtained from the distribution of the absolute values of the overlap.

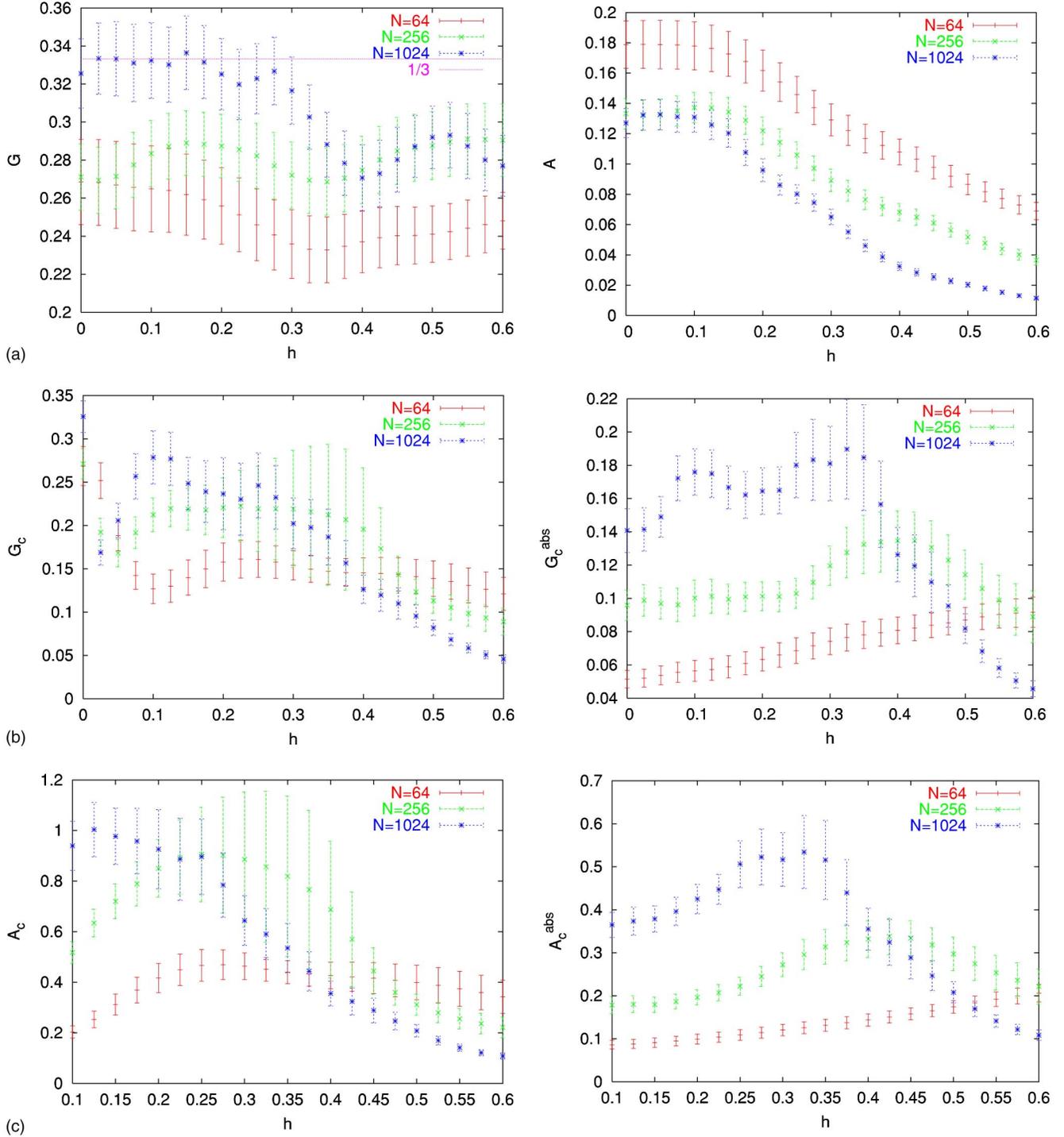


FIG. 4. The behavior of the parameters $G(h, T)$ and $A(h, T)$ (a), $G_c(h, T)$ and $G_c^{abs}(h, T)$ (b), and $A_c(h, T)$ and $A_c^{abs}(h, T)$ (c) at $T = 0.6$, as a function of the magnetic field for the different system sizes.

not coincide, but they do when finite size effects are negligible.

B. Critical behavior at the AT line

Let us now look at the dimensionless ratios of $P(q)$ moments which should intersect at $h_{AT}(T)$, providing evidences for the phase transition (Here, $h_{AT} \approx 0.382$). We present in

Fig. 3 the behavior of the Binder parameter and of the skewness. The original B and S of Eqs. (5) and (6) are on the left of the figure and the absolute variants on the right. We see that in all cases it would be a hard task to get a clear unambiguous determination of the critical point from the data. At variance with the behavior of the $h=0$ Binder parameter which is always positive and increases continuously for decreasing T 's, all four quantities in Fig. 3 (the absolute

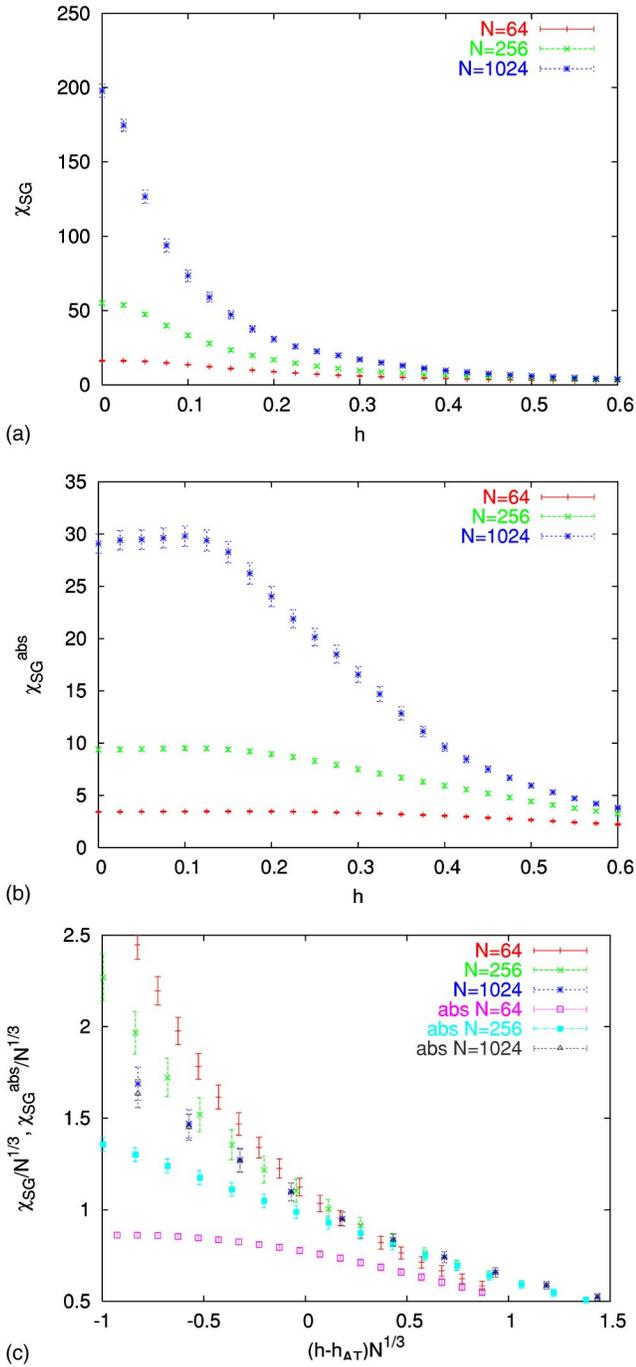


FIG. 5. (a) The behavior of the spin-glass susceptibilities $\chi_{SG}(h, T)$ and (b) $\chi_{SG}^{abs}(h, T)$. (c) Scaling plots, i.e., $\chi_{SG}(h, T)/N^{1/3}$ and $\chi_{SG}^{abs}(h, T)/N^{1/3}$ plotted as functions of the scaling variable $(h - h_{AT})N^{1/3}$ at $T=0.6$, for the different system sizes.

value does not help) display a nonmonotonic behavior, taking negative values on a large part of the interval. For B and S , the intersection between $N=256$ and $N=1024$ occurs at a definitely too small $h \approx 0.2$, showing the presence of strong finite size scaling corrections (In all cases, the value $N=64$ turns out to be too small to give interesting results). The effect of the absolute value is strong, particularly for $N=64$ and 256 . It goes in the right direction since comparing

data for $N=64$, 256 , and 1024 , we now find a monotonous crossing point behavior which approaches h_{AT} from above, with the intersection between $N=256$ and 1024 data occurring (within the error) at the correct value h_{AT} , the agreement being best in the case of the skewness.

Next, we consider in Fig. 4 the parameters based on $P(q)$ glassy phase non-self-averageness. The first observation is that in order to obtain some information one has to look at connected quantities, since G and A have definitely a different behavior from the others and do not cross as one could expect. More in detail, curves for G corresponding to $N=64$ and 256 are nearly constant (within the errors) in the whole considered h range. For $N=1024$, G is in agreement within errors with the thermodynamic limit value $1/3$ in the glassy phase, and is smaller in the paramagnetic phase. For h as large as 0.6 one still finds $G \approx 0.28$. In the case of the EA model at a fixed magnetic field, the parameter G was found to be [29] less appropriate than G_c . It decreases more slowly when entering the paramagnetic region and curves for different sizes cross at definitely too large temperatures (here quite small sizes with N between 5 and 64 were considered).

Curves for A are monotonic and approach zero (though with strong finite size corrections) at large h , making evident that $P(q)$ is self-averaging in the paramagnetic phase, but they do not cross correctly and in particular at $h=0$ one finds $A(N=1024) \approx A(N=256) < A(N=64)$.

The connected parameters display a more interesting behavior and they do indeed cross. We find a qualitatively similar behavior near the transition point for G_c and A_c . Our statistical errors are quite large and do not allow a precise determination of the crossing points, nevertheless curves for the two smaller sizes seem to roughly intersect at the correct value $h \approx 0.4 \approx h_{AT}$, whereas data for $N=256$ and 1024 appear to cross at a lower h value, this being more evident in the case of A_c . The behavior seems still better when looking at the corresponding absolute parameters. In particular, there is no irregular behavior for $h \rightarrow 0$ and the statistical errors are definitely smaller, allowing for a more precise evaluation of the crossing points. Curves corresponding to $N=64$ and 256 intersect at $h \approx 0.6$, whereas $N=256$ and 1024 clearly cross at the right value, $h \approx 0.4 \approx h_{AT}$.

To conclude the discussion on these parameters, we note that although G_c and A_c are certainly interesting to look at for obtaining evidences of the transition (and of non-self-averaging), one should not overlook their large statistical fluctuations, much larger than the fluctuations of the usual Binder parameter or the skewness, therefore a larger number of samples would be required in order to obtain precise measures.

An even better evidence for the presence of a phase transition comes from the behavior of the spin-glass susceptibility which is clearly diverging (see Fig. 5) when entering the spin-glass phase. We see that the behavior of χ_{SG}^{abs} (plotted in Fig. 5) is definitely different for the largest size considered $N=1024$ also. Here, the susceptibility seems to approach a constant in the small field region, i.e., for $h \leq h_{min}(N)$. Nevertheless, $h_{min}(N)$ clearly approaches zero for increasing

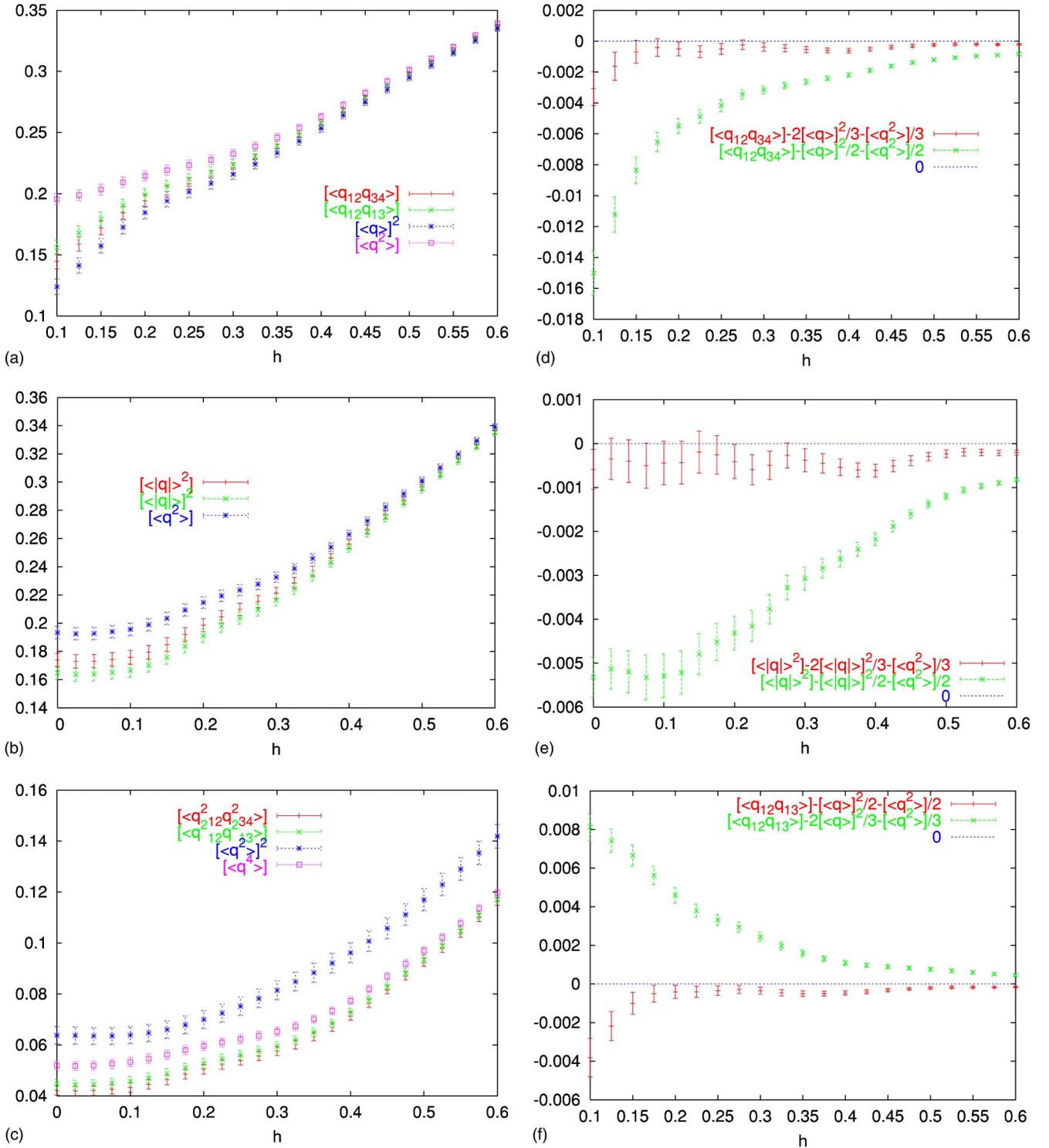


FIG. 6. We compare the behaviors of $\overline{\langle q_{12}q_{34} \rangle}$, $\overline{\langle q_{12}q_{13} \rangle}$, $\overline{\langle q \rangle}^2$, and $\overline{\langle q^2 \rangle}$ (a); $\overline{\langle |q| \rangle}^2$, $\overline{\langle |q| \rangle}^2$, and $\overline{\langle q^2 \rangle}$ (b); and $\overline{\langle q^2 \rangle}^2$, $\overline{\langle q_{12}q_{34} \rangle}^2$, $\overline{\langle q_{12}q_{13} \rangle}^2$, $\overline{\langle q^2 \rangle}^2$, and $\overline{\langle q^4 \rangle}$ (c) as functions of the magnetic field for $N=1024$. We plot (for $N=1024$ again) relations R_{1234}^a (d), $R_{1234}^{a,abs}$ (e), and R_{1213}^a (f), which are well satisfied, together with the modified ones T_{1234} , T_{1234}^{abs} , and T_{1213} , respectively, which are not in the SG phase (see text).

sizes and also in this case one gets evidence for a diverging spin-glass susceptibility.

The importance of considering both the usual χ_{SG} and the corresponding absolute quantity χ_{SG}^{abs} becomes evident when

looking at the scaling plot presented in Fig. 5. We find strong corrections to scaling in the glassy phase, such that it would be hard to evaluate the correct critical point and exponents from these data. On the other hand, corrections to χ_{SG} are in

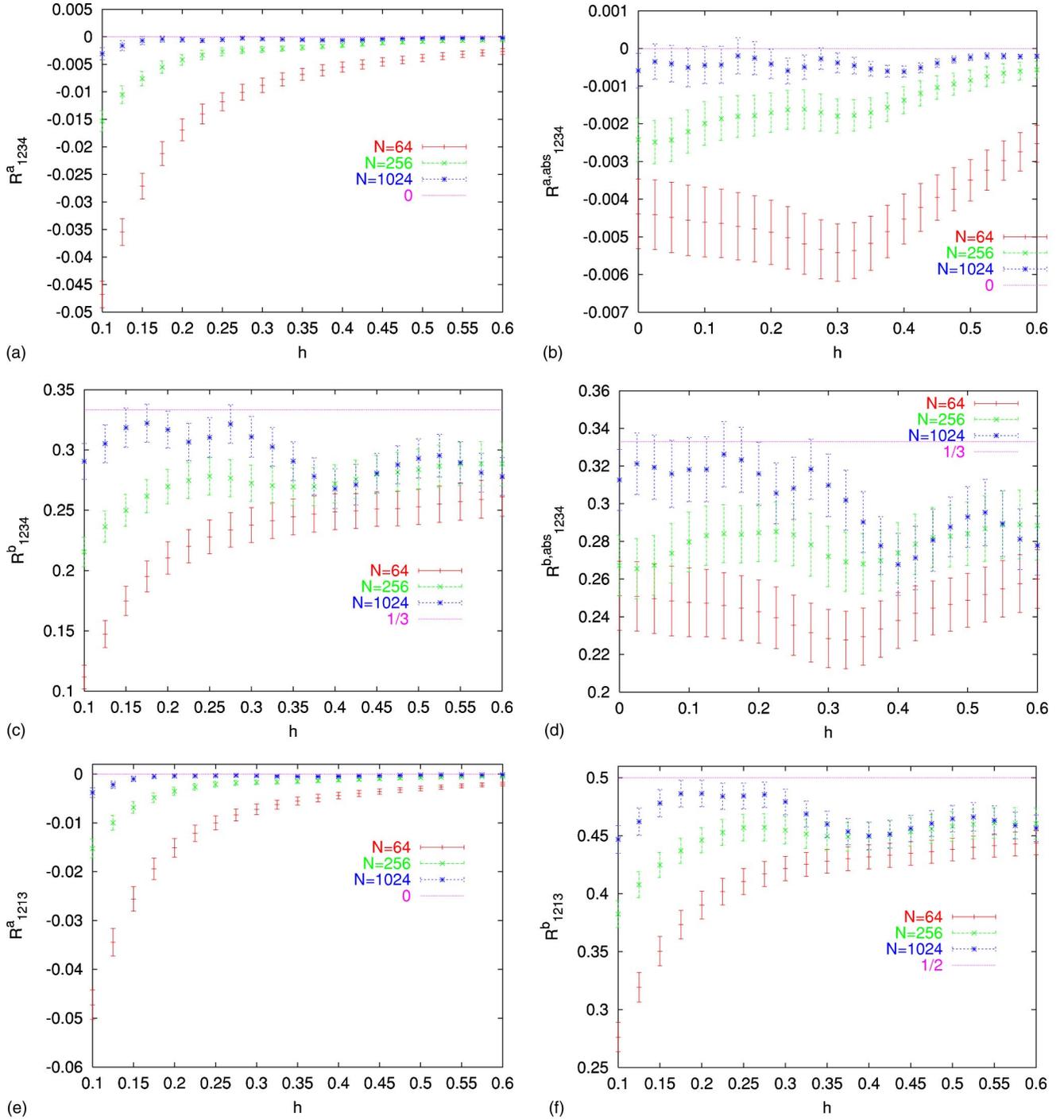


FIG. 7. The behavior of R^a_{1234} (a), $R^{a,abs}_{1234}$ (b), R^b_{1234} (c), $R^{b,abs}_{1234}$ (d), R^a_{1213} (e), and R^b_{1213} (f) as a function of the magnetic field for the different system sizes considered.

the direction opposite to those on χ_{SG}^{abs} , and therefore it is useful to look at both quantities for understanding the true scaling behavior. We also note that data for χ_{SG} and χ_{SG}^{abs} are nearly coincident in the whole relevant interval (i.e., down to $h \approx 0.3$) for $N=1024$, which means that when looking at sizes of this order or larger one can expect to find not too important corrections to scaling.

C. The sum rules

Our next aim is to investigate the validity of the stochastic stability sum rules (10)–(17). Some are supposed to be non-trivially valid for $h < h_{AT}$, and trivially valid for $h > h_{AT}$, namely, R^a_{1234} , R^a_{1213} , R^2_{1234} , and R^2_{1213} . On the other hand, relations R^b_{1234} and R^b_{1213} , which are ratio of moments, are supposed to be only valid below the AT line. We will also

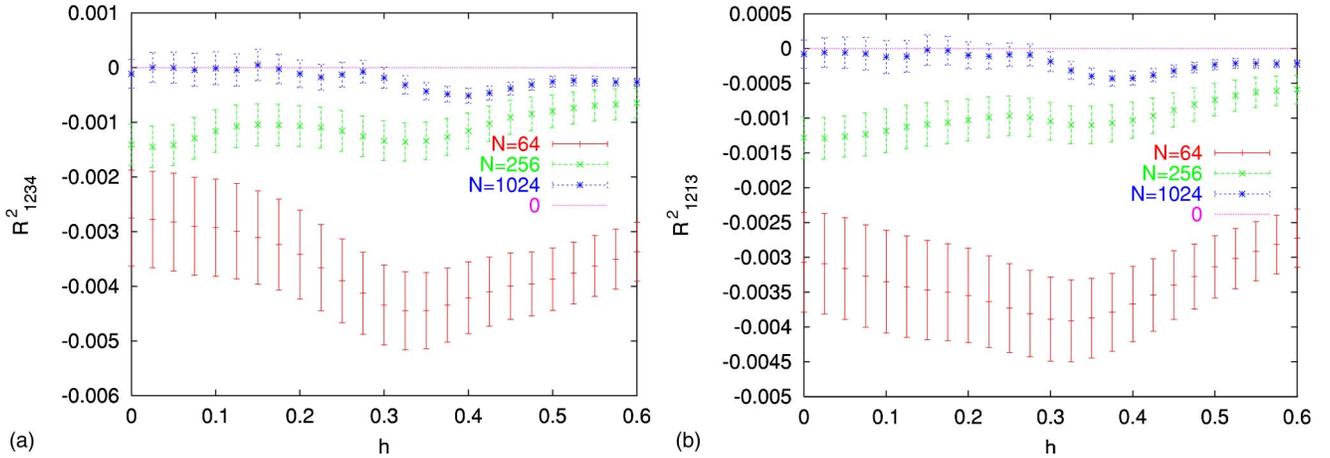


FIG. 8. (a) The behavior of R^2_{1234} and (b) R^2_{1213} as a function of the magnetic field for the different system sizes.

consider relations $R^{a,abs}_{1234}$ and $R^{b,abs}_{1234}$, obtained from the probability distribution of the absolute values of the overlap.

We first look at the behavior, as a function of the magnetic field, of the different terms entering the sum rules, considering the case of $N=1024$, where finite size corrections are less important. We see from Fig. 6 that

$$\overline{\langle q_{12}q_{34} \rangle} \approx \overline{\langle |q| \rangle^2} \approx \overline{\langle q_{12}q_{13} \rangle} \approx \overline{\langle q \rangle^2} \approx \overline{\langle q^2 \rangle} \quad (26)$$

for $h \geq 0.4$, which is quite reasonable since this is the replica symmetric region where $P(q)$ is self-averaging. The tail of $P(q)$ in the negative overlap region has practically disappeared for $N=1024$, so that $\langle q \rangle \approx \langle |q| \rangle$, and we have moreover (assuming a Gaussian distribution with variance σ^2)

$$\overline{\langle q^2 \rangle} = \sigma^2 + q_{EA}^2 \approx q_{EA}^2 = \overline{\langle q \rangle^2}. \quad (27)$$

On the other hand, these quantities are different when entering into the glassy phase, though the differences appear small.

We plot in the Fig. 6 the relations R^a_{1234} , $R^{a,abs}_{1234}$, and R^a_{1213} . In order to show that they are nontrivially verified we also, plot following Ref. [3], the relations

$$T_{1234}(h, T) = \overline{\langle q_{12}q_{34} \rangle} - \frac{1}{2} \overline{\langle q \rangle^2} - \frac{1}{2} \overline{\langle q^2 \rangle} = 0, \quad (28)$$

$$T^{abs}_{1234}(h, T) = \overline{\langle |q| \rangle^2} - \frac{1}{2} \overline{\langle |q| \rangle^2} - \frac{1}{2} \overline{\langle q^2 \rangle} = 0, \quad (29)$$

$$T_{1213}(h, T) = \overline{\langle q_{12}q_{13} \rangle} - \frac{2}{3} \overline{\langle q \rangle^2} - \frac{1}{3} \overline{\langle q^2 \rangle} = 0, \quad (30)$$

which should also be verified if R^a_{1234} , $R^{a,abs}_{1234}$, and R^a_{1213} were trivial. They are clearly not verified in the spin-glass phase, and accordingly R^a_{1234} and R^a_{1213} are nontrivial in this phase. We moreover note that to look at the probability distribution of the absolute value overlap very is useful also in this case, since as we already pointed out these relations are derived assuming an infinitesimal magnetic field which breaks the global symmetry for inversion of all the spins. As a matter of fact, relations R^a_{1234} and R^a_{1213} are no more verified as soon as $h \leq 0.15$, where the tail of $P(q)$ in the negative overlap region becomes important also for $N=1024$ (we

do not present data for $h \leq 0.1$). On the other hand, relation $R^{a,abs}_{1234}$ appears very well satisfied within the errors down to $h=0$.

In Fig. 7 we present our data for relations R^a_{1234} , $R^{a,abs}_{1234}$, and R^a_{1213} with a finer vertical scale than in Fig. 6, together with data for R^b_{1234} , $R^{b,abs}_{1234}$, and R^b_{1213} . The situation is quite clear: for $N=1024$ relations R^b_{1234} , $R^{b,abs}_{1234}$, and R^b_{1213} are not verified above the AT line, whereas they are satisfied within the statistical error below (up to crossover effects for small h 's for the non absolute quantities).

In any event, the change of behavior in the sum rules when going from the $h \leq 0.4$ region to the other side of the AT line is small. This is trivial in the case of relations R^a_{1234} , $R^{a,abs}_{1234}$, and R^a_{1213} since all terms become very similar (see Fig. 6) as we already discussed. This can be understood [50] for R^b_{1234} , $R^{b,abs}_{1234}$, and R^b_{1213} (i.e., the ratios $\chi^{1234}_{SG}/\chi_{SG} = \chi^{abs,1234}_{SG}/\chi_{abs,SG} = 1/3$ and $\chi^{1213}_{SG}/\chi_{SG} = 1/2$, respectively), using the results of Ref. [51]. These R^b 's can be calculated from the masses r_R , r_L , and $(r_L - r_A)/n$ computed in this paper. Rather surprisingly, the ratio condition becomes true again in the high field limit, and the R^b 's gain back their 1/2 and 1/3 values. This means that these R^b 's have only a very slight variation in the replica symmetric phase, with probably a minimum, and they are continuous at the AT line. We note that their behavior is very similar to the behavior of G , further confirming that appropriate parameters for getting evidence for the transition are the ones which involve connected quantities, such as G_c and A_c .

In Fig. 6 we also present the behavior of the different terms entering the relations R^2_{1234} and R^2_{1213} . $\overline{\langle q^2 \rangle^2}$ is definitely different from the other terms, and quite surprisingly it remains clearly different also on the other side of the AT line, which is to be interpreted as a reminiscence of non-self-averageness due to finite size effects.

Finally, we plot in Fig. 8 relations R^2_{1234} and R^2_{1213} . Here, finite size effects are less important because these relations are valid also in the $h \rightarrow 0$ limit. Nevertheless these quantities are compatible with zero within our statistics for $h \leq 0.3$ only for $N=1024$. Also, in this case we find only a small difference between the $h < 0.4$ behavior and the one

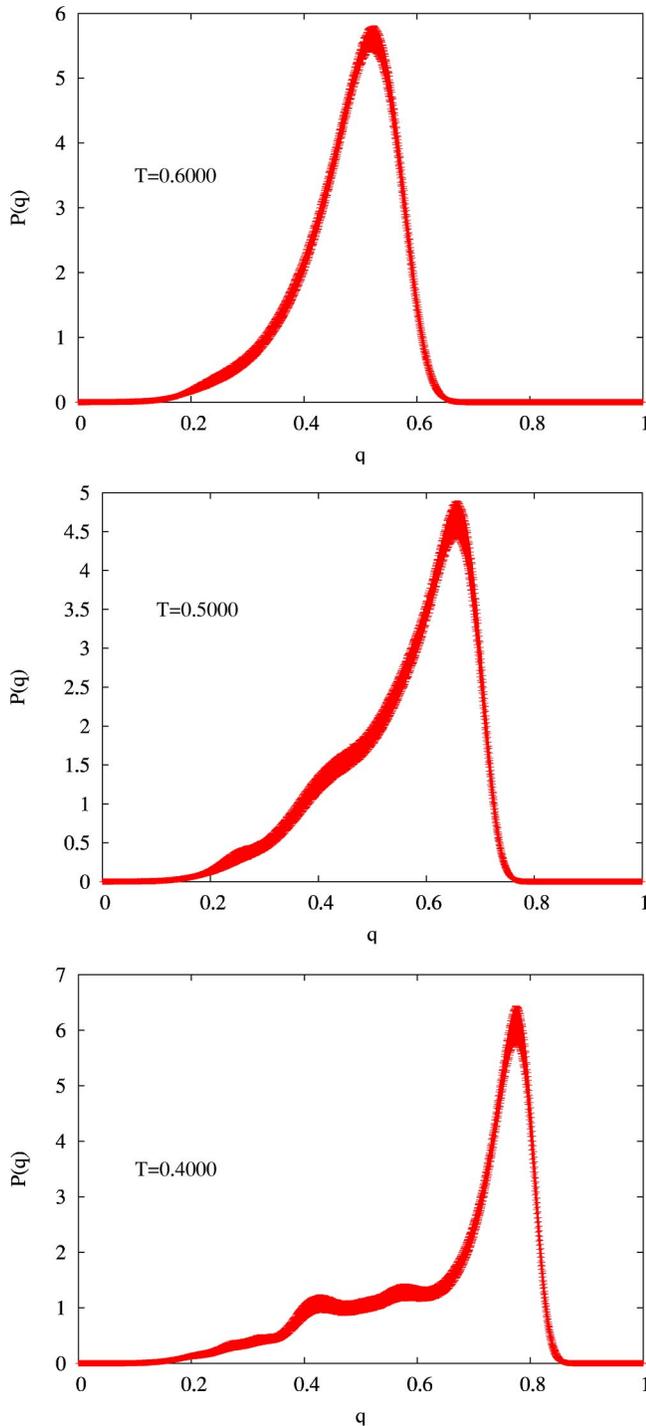


FIG. 9. The behavior of the probability distribution of the overlap $P(q)$ with $h=0.3$ and temperatures $T=0.4$, 0.5 , and 0.6 , respectively, for the large size $N=3200$.

outside the glassy phase. From this point of view, it should be recalled that $\langle q^2 \rangle^2$ is definitely different from the other terms in the whole h range, which means that data for $h > 0.4$ are far from being in the asymptotic self-averaging regime in which these sum rules should be trivially satisfied. We note that from relation R^2_{1234} the expected behavior of the parameter G immediately follows and that the small dif-

ferences we observe here between the behaviors inside and outside the glassy phase do indeed reflect the fact that G is not an appropriate observable to look at for obtaining evidence of the transition.

D. $P(q)$ for a large size

Our data for $P(q)$ at $h=0.3$ for a system of 3200 spins can be found in Fig. 9 for $T=0.4$, 0.5 and 0.6 . The corresponding values of q_{EA} are 0.759 , 0.640 , and 0.505 , respectively. We have been very careful in checking that thermalization is achieved for all values of the temperature. It is clear from the figure why the asymptotic behavior of this distribution has escaped observation up to now. At $T=0.6$ only a single peak (corresponding to q_{EA}) is visible, with substantial asymmetry (the distribution is wider in the low q side). The asymmetry is stronger for $T=0.5$, but there is still no sign of the low q peak.³ Only for $T=0.4$ does one see the expected continuum on the left of the self-overlap peak, with some indication of the low- q peak at a location in agreement with the value [46] $q_{min} \approx 0.44$. It should be noted that the peak corresponding to q_{min} is predicted to be broader than the one corresponding to q_{EA} [52]. This explains why we do not observe this minimum overlap peak.

V. CONCLUSIONS

We performed numerical simulations of the SK model in a magnetic field at temperature $T=0.6$, both in the glassy phase and above the AT line. We used a modified version of the PT algorithm in which the system is allowed to move between a chosen set of magnetic field values, an algorithm well suited for our purpose.

We measured quantities such as the magnetic susceptibility, which turns out to be in agreement with the predicted analytical behavior of Ref. [47] as a function of h .

Dimensionless ratios of $P(q)$ moments such as the Binder parameter and the skewness display a nonmonotonic behavior, making it difficult to get a clear determination of the transition point on the AT line. Also *ad hoc* parameters for locating replica symmetry breaking transitions, based on the non-self-averageness of the order parameter, are considered. The connected ones turn out to be effective for locating the transition.

An even better evidence for the transition comes from the divergence of the spin-glass susceptibility, though its scaling behavior is affected by strong finite size corrections.

We also investigate the behavior of various quantities defined in terms of the probability distribution of the absolute value of the overlap. This allows one to reduce the finite size effects due to the long tail of $P(q)$ in the negative overlap region. As a matter of fact, the dimensionless parameters turn out to behave better in this case, the crossing points being nearer to the correct critical value. It is interesting to note

³This result disagrees with Ref. [16], where a low q peak is found, using the Metropolis algorithm with 100 000 sweeps for equilibrium and only 20 disorder samples.

that the usual and absolute susceptibilities have corrections of opposite signs.

Moreover, we studied the behavior of some sum rules (related to stochastic stability) involving overlaps between three and four replicas. We found strong finite size corrections particularly for those sum rules that are valid only at a nonzero magnetic field, and it turns out to be particularly appropriate to look at absolute quantities in this case. They are satisfied within our statistical accuracy for $N=1024$ in the glassy phase. On the other hand, they would not be good indicators for the transition, since their behaviors change very slightly when crossing the AT line, being still nearly verified also for $h > h_{AT}$, some trivially (all the terms become very similar) and others nontrivially.

Finally, we presented data for $P(q)$ in the magnetic field,

which show how slowly the shape predicted by the RSB solution develops on a large system.

ACKNOWLEDGMENTS

We are particularly grateful to Giorgio Parisi for many interesting discussions and useful suggestions. We would like to thank Tamas Temesvári for pointing to us an error in the original manuscript and for many discussions. We also acknowledge discussions with Andrea Crisanti, Cirano De Dominicis, Enzo Marinari, Felix Ritort, Tommaso Rizzo, and Peter Young. B.C. was supported by the European Union. We thank Andrea Crisanti and Tommaso Rizzo for providing us with their unpublished results on the $h \neq 0$ SK model.

-
- [1] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975).
- [2] G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979); J. Phys. A **13**, 1101 (1980); **14**, 1887 (1980); **13**, L115 (1980).
- [3] For a review see E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. Ruiz-Lorenzo, and F. Zuliani, J. Stat. Phys. **98**, 973 (2000).
- [4] M. Mézard, G. Parisi, and M.A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore 1987).
- [5] K. Binder and A.P. Young, Rev. Mod. Phys. **58**, 801 (1986).
- [6] J.R.L. De Almeida and D.J. Thouless, J. Phys. A **11**, 983 (1978).
- [7] W.L. McMillan, J. Phys. C **17**, 3179 (1984).
- [8] A.J. Bray and M.A. Moore, J. Phys. C **18**, L699 (1985).
- [9] D.S. Fisher and D.A. Huse, Phys. Rev. B **38**, 386 (1988).
- [10] N. Sourlas, Europhys. Lett. **1**, 189 (1986).
- [11] S. Caracciolo, G. Parisi, S. Patarnello, and N. Sourlas, Europhys. Lett. **11**, 783 (1990); J. Phys. (France) **51**, 1877 (1990); D.A. Huse and D.S. Fisher, J. Phys. I **1**, 621 (1991); S. Caracciolo, G. Parisi, S. Patarnello, and N. Sourlas, *ibid.* **1**, 627 (1991).
- [12] E.R. Grannan and R.E. Hetzel, Phys. Rev. Lett. **67**, 907 (1991).
- [13] N. Kawashima, N. Ito, and M. Suzuki, J. Phys. Soc. Jpn. **61**, 1777 (1992); N. Kawashima and N. Ito, *ibid.* **62**, 435 (1993).
- [14] D. Badoni, J.C. Ciria, G. Parisi, F. Ritort, J. Pech, and J.J. Ruiz-Lorenzo, Europhys. Lett. **21**, 495 (1993).
- [15] J.C. Ciria, G. Parisi, F. Ritort, and J.J. Ruiz-Lorenzo, J. Phys. I **3**, 2207 (1993).
- [16] M. Picco and F. Ritort, J. Phys. I **4**, 1619 (1994).
- [17] M. Picco and F. Ritort, Physica A **250**, 46 (1998).
- [18] G. Parisi, F. Ricci-Tersenghi, and J.J. Ruiz-Lorenzo, Phys. Rev. B **57**, 13 617 (1998)
- [19] E. Marinari, G. Parisi, and F. Zuliani, J. Phys. A **31**, 1181 (1998).
- [20] E. Marinari, C. Naitza, and F. Zuliani, J. Phys. A **31**, 6355 (1998).
- [21] J. Houdayer and O.C. Martin, Phys. Rev. Lett. **82**, 4934 (1999); E. Marinari, G. Parisi, and F. Zuliani, *ibid.* **84**, 1056 (2000); J. Houdayer and O.C. Martin, *ibid.* **84**, 1057 (2000).
- [22] F. Krzakala, J. Houdayer, E. Marinari, O.C. Martin, and G. Parisi, Phys. Rev. Lett. **87**, 197204 (2001).
- [23] J. Lamarcq, J.-P. Bouchaud, and O.C. Martin, e-print cond-mat/0208100.
- [24] A. Cruz, L.A. Fernandez, S. Jiménez, J.J. Ruiz-Lorenzo, and A. Tarancón, e-print cond-mat/0209350.
- [25] I.R. Pimentel, T. Temesvári and C. De Dominicis, Phys. Rev. B **65**, 224420 (2002); T. Temesvári and C. De Dominicis, Phys. Rev. Lett. **89**, 097204 (2002).
- [26] F. Ritort, Phys. Rev. B **50**, 6844 (1994).
- [27] A. Billoire and B. Coluzzi, Model. Phys. Rev. E (to be published), e-print cond-mat/0210489.
- [28] E. Marinari, C. Naitza, F. Zuliani, G. Parisi, M. Picco, and F. Ritort, Phys. Rev. Lett. **81**, 1698 (1998); H. Bokil, A.J. Bray, B. Drossel, and M.A. Moore, *ibid.* **82**, 5174 (1999); E. Marinari, C. Naitza, F. Zuliani, G. Parisi, M. Picco, and F. Ritort, *ibid.* **82**, 5175 (1999).
- [29] F. Ritort and M. Sales, J. Phys. A **33**, 6505 (2000); **34**, L333 (2001); M. Picco, F. Ritort, and M. Sales, Eur. Phys. J. B **19**, 565 (2001); F. Ritort and M. Sales, J. Phys. A **34**, L333 (2001).
- [30] A.P. Young, A.J. Bray, and M.A. Moore, J. Phys. C **17**, L149 (1984).
- [31] M. Mézard, G. Parisi, N. Sourlas, G. Toulouse, and M.A. Virasoro, J. Phys. (France) **45**, 843 (1984).
- [32] F. Guerra, Int. J. Mod. Phys. B **10**, 1675 (1996).
- [33] S. Ghirlanda and F. Guerra, J. Phys. A **31**, 9149 (1998).
- [34] M. Aizenman and P. Contucci, J. Stat. Phys. **92**, 765 (1998).
- [35] P. Contucci, e-print math-ph/0205041.
- [36] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
- [37] R.N. Bhatt and A.P. Young, Phys. Rev. Lett. **54**, 924 (1985).
- [38] G. Parisi, Proceedings of the Conference Disordered and Complex Systems, London, 2000 (unpublished), e-print cond-mat/0007347.
- [39] E. Marinari, G. Parisi, J.J. Ruiz-Lorenzo, and F. Ritort, Phys. Rev. Lett. **76**, 843 (1996).
- [40] E. Marinari and F. Zuliani, J. Phys. A **32**, 7447 (1999).
- [41] G. Parisi, M. Picco, and F. Ritort, Phys. Rev. E **60**, 58 (1999).
- [42] K. Hukushima and H. Kawamura, Phys. Rev. E **62**, 3360 (2000)
- [43] M. Campellone, B. Coluzzi, and G. Parisi, Phys. Rev. B **58**, 12 081 (1998).

- [44] B. Drossel, H. Bokil, and M.A. Moore, Phys. Rev. E **62**, 7690 (2000).
- [45] 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**, 14 237 (2000).
- [46] A. Crisanti and T. Rizzo, e-print cond-mat/0111037; (private communication).
- [47] G. Parisi, J. Phys. A **13**, 1887 (1980).
- [48] G. Parisi and G. Toulouse, J. Phys. (France) Lett. **41**, L361 (1980).
- [49] A. Crisanti, T. Rizzo, and T. Temesvári, e-print cond-mat/03002538.
- [50] T. Temesvári (private communication).
- [51] I.R. Pimentel, T. Temesvári, and C. De Dominicis, Eur. Phys. J. B **25**, 361 (2002).
- [52] S. Franz, G. Parisi, and M.A. Virasoro, J. Phys. I **2**, 1869 (1992).