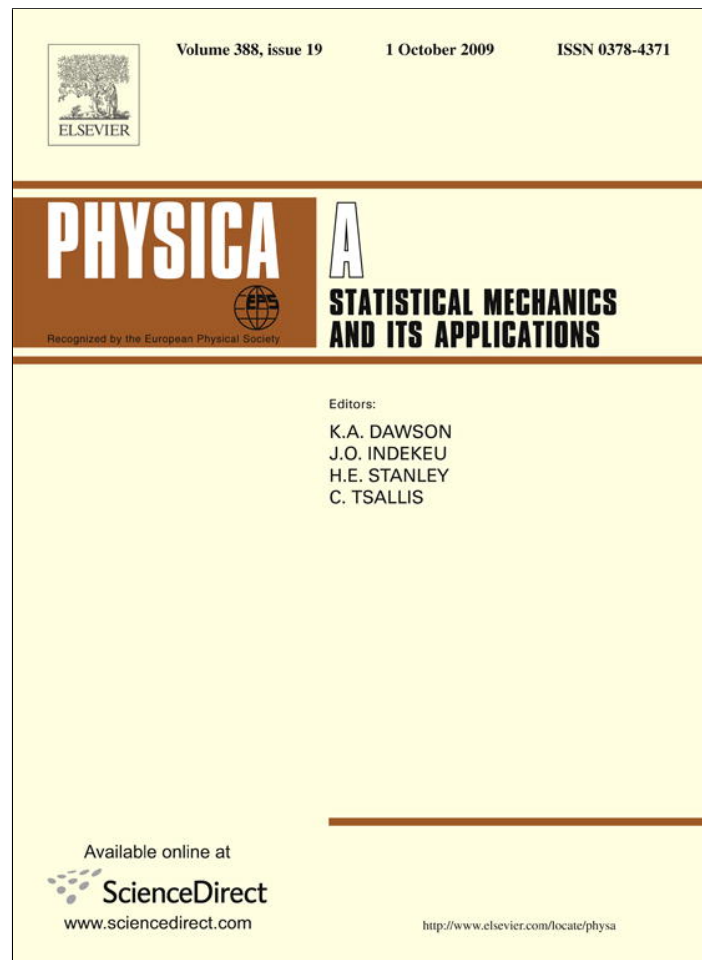


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Phase transitions in Edwards–Anderson model by means of information theory

E.E. Vogel^{a,*}, G. Saravia^a, F. Bachmann^a, B. Fierro^b, Janine Fischer^c

^a Physics Department, Universidad de La Frontera, Casilla 54-D, Temuco, Chile

^b Physics Department, Universidad Santa María, Valparaíso, Chile

^c Technische Universität, Dresden, Federal Republic of Germany

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ABSTRACT

A numeric method to characterize phase transitions is presented, explained and applied to a two-dimensional disordered system that can be thought of as a diluted ferromagnet or an Edwards–Anderson model near the ferromagnetic limit. A computer simulation is implemented to define a time series for order parameters; a file stores the time evolution of each parameter for different dilution concentrations and for a series of temperatures. These files are compressed and they reach a maximum size for temperatures in agreement with critical temperatures for the ferromagnetic/paramagnetic transition obtained by other methods. Site order parameter gives optimum results for this method based on data compression. Data compression procedures are invoked to give a qualitative explanation of this phenomenon. The advantages of this method are discussed by comparing results and procedures with two established methods: the crossing of Binder cumulants and the crossing of time autocorrelation functions. Other possible applications and extensions of this method are also mentioned.

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1. Introduction

A very well established method to characterize phase transitions for systems such as the Edwards–Anderson model in 2 dimensions (2D) is to look for the Binder cumulant (BC) as a function of temperature: curves for different sizes all cross at the critical temperature (T_C) [1]. It was recently reported that a similar treatment can also be done by looking at the crossing of autocorrelation functions for an order parameter, eventually the same one used to define the BC [2].

In the present paper we present an alternative way to find the critical temperature for a phase transition based on the information content of the file storing an order parameter characterizing such phase transitions. In a way, we came across this empiric result when doing the previously mentioned study concerning autocorrelation functions as we were forced to do long routines of calculations and store huge amount of results. Compressing numerous files was unavoidable. It turns out that the size of the compressed file is a function of the temperature of the simulation, thus opening a new line of research whose initial results are reported here.

We will show how the size of the compressed file maximizes at a temperature T_M slightly over T_C . Moreover, the dependence of T_M on the size of the systems shows the expected tendency towards the thermodynamic limit. Then, the analysis of the size reached by compressed files concerning order parameters of a system becomes a novel, easy to use and fast method to study phases and critical phenomena, independent and complementary to other existing methods. All of this

* Corresponding author. Tel.: +56 45 325316; fax: +56 45 325323.

E-mail address: ee_vogel@ufro.cl (E.E. Vogel).

Table 1

Summary of the number of samples used for each value of x (concentration of antiferromagnetic bonds). This distribution holds for each lattice size L .

x	Number of samples
0.0	1
0.015625	4
0.031250	8
0.046875	16
0.062500	32
0.078125	32
0.093750	32
0.109375	32
0.125000	32

is based on numeric experiments involving long computer times and storage of large amount of data. Results reflect clear accepted tendencies upon variation of three independent variables: temperature, disorder in the system and lattice size. We will refer to this new way of detecting transition temperatures as the *file compression* (FC) method. A theoretical description is far beyond the scope of the present article, however, we do include some justification based on the way data compressors work.

In the next section we present the methodology used to generate and compress the data files, analyzing the main results. Section 3 is devoted to draw conclusions and venture possible future lines of action and applications.

2. Methodology and results

Let us review the procedure aimed to obtain the data. Although the methodology presented here can be generalized to any system, we will consider the bimodal Edwards–Anderson model [3] on a square lattice. This system has been around for three decades, still challenging theory and computer capabilities [4]. We will review here its features that are most directly connected to the present study. The Hamiltonian can be written as

$$H = \sum_{i < j} J_{ij} S_i S_j \tag{1}$$

where J_{ij} is the exchange interaction between nearest-neighbor spins at sites i and j respectively, which can be either ferromagnetic (F, $J_{ij} = -J$; $J > 0$) or antiferromagnetic (A, $J_{ij} = J$). The latter is randomly distributed through the sample with concentration x . Since the aim of the present paper is to concentrate on a well defined phase transition we will focus on a range of small values of x , where a ferromagnetic to paramagnetic transition is found as temperature is raised. Due to the symmetry of the Hamiltonian with respect to the point $x = 0.5$, the same results should be obtained for large values of x (approaching 1.0). For the range $0.1 < x < 0.9$, roughly speaking, no such a phase transition is obtained and a spin glass to paramagnetic transition exists only at zero temperature. A recent phase diagram containing this information has been recently proposed [5].

Let us begin by considering a lattice size $L \times L$ in the range of study: from 8×8 to 128×128 (largest size is limited by the effective CPU time used); in practice we speak of 5 different sizes under consideration: 8×8 , 16×16 , 32×32 , 64×64 , and 128×128 . For each size, we define a concentration x at intervals of $\delta x = 1/64 = 0.015625$, which means the following 9 values for the AF concentrations were used for this study: 0.0, 0.015625, 0.03125, 0.046875, 0.0625, 0.078125, 0.09375, 0.109375, and 0.125. Reasons for stopping at this last value have to do with previously referred phase diagram and they will be clear in the discussion. Just one F sample ($x = 0.0$) is representative for the class. As x increases more realizations are possible, so several samples must be prepared to have a set representative for the class. A summary of the samples used here is presented in Table 1.

For any sample a temperature T (measured in units of J) is defined. Evolution is now done invoking a Monte Carlo (MC) procedure with Metropolis algorithm [6,7]; time t is measured in MC steps (MCS) and a state of the system is given by the instantaneous orientation of the spins at all sites $S_i(t)$. Each temperature defines one separate run of the simulations. Temperatures will be varied at intervals of $dT = 0.01$ to well detect the phase transition.

Several observables can be measured as functions of time: energy, neighbor correlations, magnetization, site order parameter, susceptibilities and specific heat. For the purposes of this work we focus on two parameters. The magnetization per site can be defined as:

$$\mu(t) = \frac{1}{N} \sum_{i=1}^N S_i(t). \tag{2}$$

We will pay particular attention to the absolute value of the Edwards–Anderson site order parameter defined as

$$q(t) = \frac{1}{N} \left| \sum_{i=1}^N S_i(0) S_i(t) \right|, \tag{3}$$

where $S_i(0)$ is the set of spin orientations at an initial state in the way defined below.

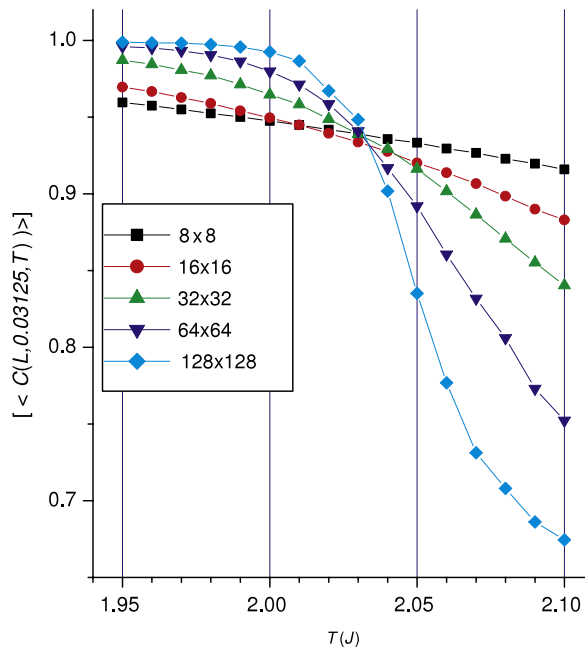


Fig. 1. Average time correlation functions for $x = 0.03125$ as function of temperature for the lattice sizes displayed in the inset. All curves cross at $T = T_c \approx 2.03$ (in units of J), corresponding to the critical temperature for the spin glass transition. Crossing temperatures for other concentrations can be obtained in a similar way.

The outcome of this process for the m th sample of size $L \times L$, concentration x , at temperature T , are sets of sequential data in time, that can be stored as vectors $\mu_m(L, x, T, t)$, $q_m(L, x, T, t)$ and so on.

The time evolution is done in the following way. An initial state (orientation of all Ising spins) is randomly chosen and equilibration at temperature T is let to evolve during 1000 MCS. Then the initial time $t = 0$ is defined, and state $S_i(0)$ is defined and stored. We concentrate here on the previously defined parameters $\mu(t)$ and $q(t)$. It will turn out that the latter shows the best definition among all the studied parameters. Magnetization will be included up to the point we compare its results with those of the q parameter.

After $t = 0$, evolution continues and values of the parameter $q(t)$ are now stored every 20 MC steps (for no particular reason other than avoiding huge files). The process is stopped arbitrarily after 120,000 of such instants, needing a total of 2,400,000 MCS. This is done for each T , for each x and for each L , meaning both a large amount of CPU time used and a large amount of stored data.

Then time autocorrelation functions can be calculated to assess the time evolution of any order parameter, such as $q(t)$. We use the following form for the autocorrelation function [2]:

$$C(\tau) = \frac{\nu}{\nu - \tau} \frac{\sum_{\ell=0}^{\nu-\tau} \sum_{\ell=0}^{\nu-\tau} q(\ell)q(\ell + \tau)}{\sum_{\ell=0}^{\nu} q(\ell)^2} \quad (4)$$

where τ is the lapse separating the two instants that are compared through the entire file comprising ν instants.

Average values $[\langle C(L, x, T) \rangle]$ of time autocorrelation functions (TAF) are obtained for each triad: L , x and T . Notice that this is a double average: first is an average $\langle . \rangle$ over τ through the entire time window on each sample, then it is an average $[.]$ over all samples in the class.

The critical temperature T_c can be obtained by means of the crossing of TAF, when plotting $[\langle C(L, x, T) \rangle]$ for different L values as function of temperature [2]. This is shown in Fig. 1, for $x = 0.03125$, where it can be seen that curves for different sizes all cross at $T = T_c \approx 2.03$. A report showing that the crossings of TAF yield results that are equivalent to those obtained by means of crossings of BC was presented in Ref. [2] using smaller samples. Fig. 1 shows how the method stabilizes for larger sizes. We use TAF from now on as a basis for comparison for the results coming from the method of data compression introduced below.

Let us now go back to the instance in which a file, $q_m(L, x, T, t)$ say, has been stored. Then a data compressor or zipper is invoked to generate a compressed file, which we designate by $\tilde{q}_m(L, x, T)$. Almost any data compressor serves for the general purposes of the present paper. We have chosen the compressor known as bzip2, based on the Burrows Wheeler algorithm, since it is in public domains, it is open source and has given a consistently good response for all the data analyzed here. This compressor shows a good compression ratio approaching the optimum defined by Shannon's information theory [8,9].

For the purposes of this paper the weight or size of the files is conveniently measured in kilobytes (kB). Let us designate by $W_m(L, x, T)$ the size of $\tilde{q}_m(L, x, T)$. The average weight over all files correspondingly to samples of the same class is denoted

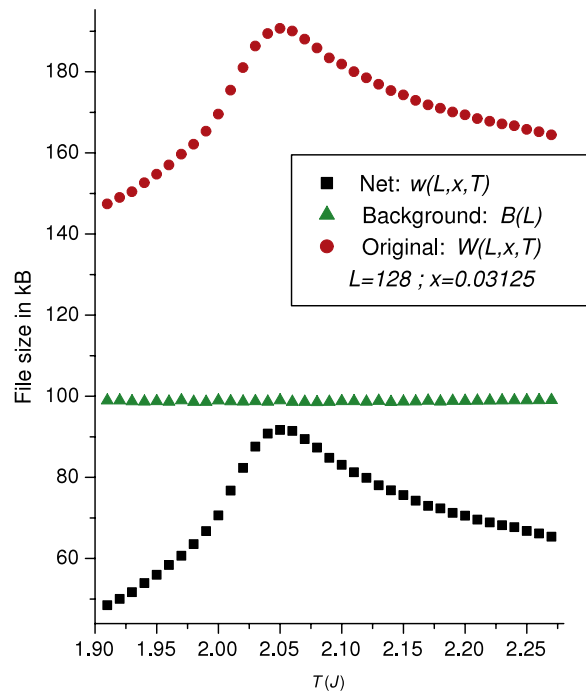


Fig. 2. Average weight $W(L, x, T)$ of file for order parameter $q(L, x, T)$ for concentration $x = 0.03125$ and lattice size $L = 128$; file size for q parameter corresponding to an empty lattice of same size $B(L)$. The difference is the net file size $w(128, 0.03125, T)$ which will be studied by varying lattice size and concentration.

by $W(L, x, T)$. Part of this weight is exclusively due to the lattice size and it is convenient to separate this component out to compare the role of compression under different temperatures equilibrating with the internal interactions. This is accomplished by running an empty lattice (no interactions) for each L getting a file for the value of the parameter; the corresponding compressed file for q has a weight $B(L)$. Then, $w(L, x, T)$, the net weight of the compressed file due to the internal interactions is given by

$$w(L, x, T) = W(L, x, T) - B(L). \tag{5}$$

This process is depicted in Fig. 2 for $L = 128$ and $x = 0.03125$. The background weight $B(L)$ for parameter q corresponding to each size $L = 8, 16, 32, 64$ and 128 are 44.75, 60.03, 68.9, 83.6 and 98.8 kB respectively.

Net weight functions $w(L, x, T)$, for $x = 0.03125$, are plotted in Fig. 3 as functions of temperature T , for different lattice sizes. In all of them a maximum is reached, whose temperature T_M moves to lower values as the size of the system increases. Curves get narrower in the apex as lattice size increases. There is a clear indication for convergence for the temperature at which curves maximize towards the thermodynamic limit.

A similar analysis can be done with any observable but we found advantages when dealing with parameter q . To support this statement let us present a similar treatment for the magnetization $\mu(L, 0.03125, T)$. Again an empty lattice is run to subtract the size background noise on magnetization (different than for q) and the net weight for magnetization files is obtained; we designate by $u(L, x, T)$ such result. All of this is done in perfect analogy to Eq. (5) and Fig. 2. The results are shown in Fig. 4.

Upon comparing Fig. 3 to Fig. 4 it is clear that parameter q leads to better contrast between compressed files at the maximum with respect to the rest of the curve. Namely, maxima for q are better defined than maxima for μ , as can be seen from the curvature in upper part of corresponding curves for each parameter. Moreover, curves for q are also smoother than the corresponding curves for μ . Other parameters like energy or neighbor correlations are less sensitive than the site order parameter q (or even μ) when using the compression method. These are the main reasons we continue the analysis with q only.

Why the files of compressed $q(t)$ values become less compressible near the transition temperature? This has to do with information theory and this brings this point beyond the aim of the present paper where we want to present these numerical experiments as empirical results. However, a general explanation can be attempted based on the philosophy under which data compressors work.

Burrows Wheeler algorithm, as all data compressors, search for repeated patterns within a file, for a given width of data. Let us begin by considering the vector in the file as composed of the same value (x say) as the unique result; such monotonous file will have the highest possible compression. If the vector has the first half with the repeated value x and the second half with repeated value y such file will be less compressible than previous one but still it will be highly compressible. If the same length of x 's and y 's is alternated in regular portions within the vector the compression decreases even more. If now the length for each portion of x 's and b 's is random, compression decreases even more. Finally if many more values come

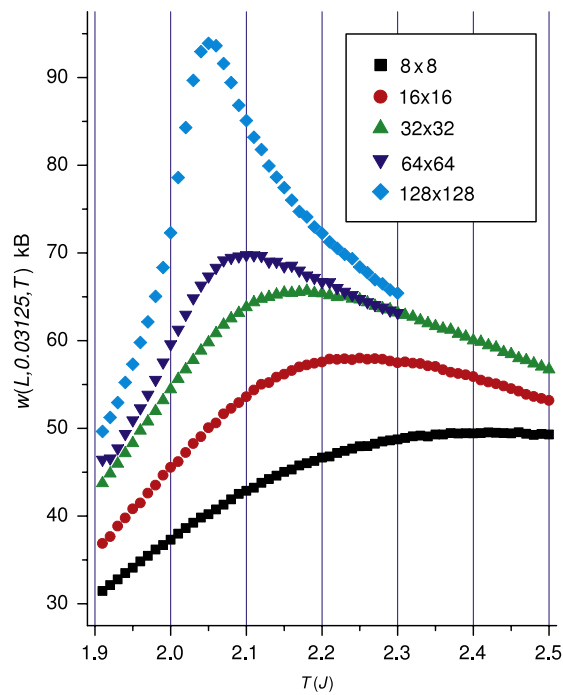


Fig. 3. Average net file size $w(L, 0.03125, T)$ for the sizes shown in the inset.

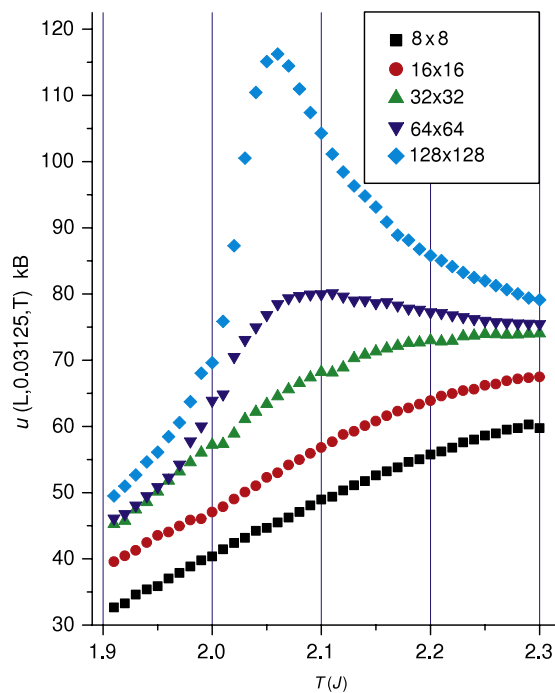


Fig. 4. Average net file size $u(L, 0.03125, T)$ for the sizes shown in the inset.

into play compression becomes increasingly difficult. For a chaotic situation, where values, portions and alternations for these values in the vector are not related to previous history, minimum compression can be expected.

The system under consideration is characterized by a discrete energy spectrum at intervals of $\delta = 4J$ (or $8J$ for the pure F case at zero temperature). We could label increasing energies in as $E_0 = 0, E_1, E_2, \dots, E_n$. The probability P_α for a state of energy E_α to be occupied is given by the Boltzmann factor: $\exp(-E_\alpha/T)$ (considering energies and temperatures measured in units of J).

At extremely low temperatures the system is trapped in a ground level, eventually evolving among the degenerate states belonging to the same energy valley. Such states are genetically connected so observables do not change much, usually repeating a few values all the time. The vector storing any observable will be monotonic and the file will be highly compressible. As temperature increases, excited states are visited making more diverse the set of values found for the

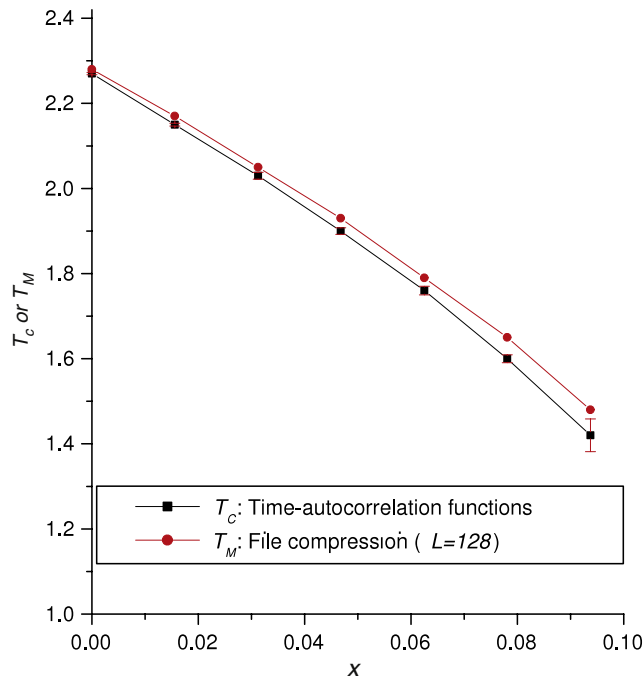


Fig. 5. Critical temperatures for size 128, at different concentrations x using crossing of the time autocorrelation function (T_c , squares) and data compression (T_M , circles).

observables. A more important change is achieved when thermal excitations overcome energy barriers allowing to reach states belonging to other energy valleys.

At extremely high temperatures all states are equally possible and order parameters as those discussed above tend to vanish. This is so since the density of states for the system under consideration maximizes for half of the spins up and half of the spins down in a random way. Divergences from nil values are of the order of $1/N$ (inverse of the number of spins) which tends to zero in the thermodynamic limit. So the vector for such an observable will be a succession of zero values (or very close to zero) making the file highly compressible. As temperature is lowered for extremely high temperatures, deviations from zero begin to appear as the system will try to spontaneously break ergodicity at low temperatures. This will make the file less compressible.

In the intermediate region both of these mechanisms contribute to a random succession of values in the vector giving account of the evolution of the observable. There is a point at which the compression is less possible which is the critical condition under which the system reaches its maximum chaotic behavior. This critical condition will depend on the lattice disorder (concentration x), so the critical temperature is expected to decrease with increasing x .

Let us apply previous reasoning to $w(128, 0.03125, T)$ which is the highest curve presented in Fig. 3, maximizing at $T_M \approx 2.05$, slightly over T_c , the crossing temperature previously found using TAF. It can be noticed that the slopes on the low-temperature side are steeper than in the high-temperature side; this is so since the mechanisms are quite different for these two temperature regimes. As we move from the maximum to lower temperatures the systems freezes in fewer energy valleys visiting states that tend to be genetically connected giving similar non-zero values for the observable, thus lowering the information content in the file. As temperature is further lowered the backbone of rigid bonds in the lattice [10] becomes more difficult to be flipped so very few spins can change leading to very few values available for the observable, which means repetitive information in the data file which makes it highly compressible. On the other hand, as we move from the maximum to high temperatures, namely, for $T \gg T_c$ interactions are overcome by thermal agitation (or interactions tend to vanish) which ends up making all states nearly equally likely, q parameter tends asymptotically to zero producing an erratic low-amplitude sequence in the parameter, which produces a file with slowly decreasing amount of information content. This last mechanism is responsible for the smooth decay of the curve towards the right-hand side. The two different mechanisms explain the non-symmetric nature of curves in Fig. 3.

A similar procedure is applied for other concentrations. Naturally, computer times increase enormously with size, so we had to stop at $L = 128$. Let us obtain the temperatures at which different $w(L, x, T)$ maximize and compare them to the critical temperatures found using TAF. This is done in Fig. 5, where it can be seen that the FC method yields results that are equivalent to those of TAF which, in its own turn, are equivalent to BC [2]. Fig. 5 stops at $x \approx 0.1$ since error bars using TAF increase with tendency to diverge for larger values of the concentration x .

In Fig. 6 we show how T_M varies with x , for $L = 128$. The stability of the curve is lost over $x = 0.1$ as it can be seen from three different features: (a) The maxima for the file sizes decrease almost linearly from $x = 0.0$ to $x = 0.09375$, while the descent is more pronounced for larger concentrations; (b) Curves become considerable broader for $x > 0.09375$; (c) The monotonic behavior of successive points in the curves up to $x = 0.09375$ is lost, so for larger concentrations oscillations

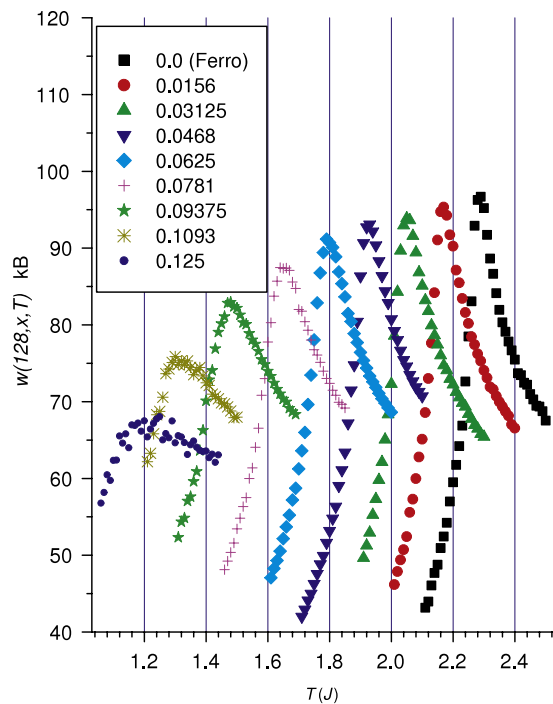


Fig. 6. Size of compressed files $w(128, x, T)$ for size 128 at different concentrations. It shows how the maxima vary with temperature and how the curves loose definition for $x > 0.10$.

are clearly appreciated as temperature is varied. Then, for $x > 0.1$ it is nearly impossible to define a unique temperature at which the curve maximizes. This fact agrees with the divergent error bars mentioned above for TAF also observed in the case of BC.

In addition to previous studies the connected susceptibility was also measured (not shown here) to see if there was a close relationship to the above figures. Except for yielding the same critical temperature (as other measurable quantities) curves are clearly different. This is so because susceptibility measures the fluctuations of a quantity with respect to its average value, where the amplitude of these fluctuations play the most important role. In the data compression method exact matching of the digital data is searched for, regardless of the amplitude of the deviations of data.

3. Discussion and conclusions

We have established that the sizes of compressed files for order parameters characterizing a phase transition reach maxima at temperatures T_M in excellent agreement with the critical temperatures T_C for the same transitions obtained by other theoretical methods (crossing of time autocorrelation functions and crossing of Binder cumulants). This is particularly true for the absolute value of the Edwards–Anderson parameter q defined in Eq. (2). The maximum size of a compressed file is determined by the increase in information content near the crossover point between two regimes. In the low T side the system tends to be trapped in one or few energy valleys, switching among genetically connected states, thus yielding similar values for the parameter, which makes the file highly compressible. In the high T side more and more states become available yielding values for the parameter near its thermal noise, thus yielding erratic similar small values for the parameter and the file becomes moderately compressible.

The process of finding of $T_M \approx T_C$ has been followed up varying x , the concentration of A bonds, in Edwards–Anderson model and it holds for $0.0 \leq x < 0.10$, where a ferromagnetic to paramagnetic transition is possible. Beyond this point all methods fail to give account of any phase transition, phenomenon which is also shown by the method of data compression that we are presenting here.

All this evidence shows that the determination of critical temperatures of phase transitions by means of the size of the compressed file associated to order parameters yields results that are equivalent to more elaborate methods. This is at least so in the case of multiple phase transitions presented here. There are also advantages for this method over the crossing methods.

Let us compare the way the three methods work to appreciate advantages and disadvantages. For any given temperature the three methods (BC, TAF, and FC) require equilibration in a thermal bath, which we take it to be the same for the three of them. Then, BC method is based on repeated measurements of the order parameter to obtain a fairly representative distribution function for the order parameter at different temperatures. The TAF method needs a sequential measurement of the order parameter to get a representative time series for the order parameter at different temperatures.

Further work needs to be done in the cases of the crossing methods. In the case of BC, the knowledge of the distribution function allows the calculation of the second and fourth momenta of the order parameter and then the BC can be calculated.

In the case of TAF, the knowledge of the vector for the order parameter allows the calculation of the time autocorrelation function. However, for any of these crossing methods the procedures must be repeated for several sizes, since it is necessary to find the actual crossing points for curves obtained at different sizes. On the contrary, in the case of the FC method just one of these sizes (naturally the largest size) is enough to approximately determine the critical temperature, corresponding to the point in which the compressed file reaches a maximum size.

Relationships between information theory and other branches of science have been unfolding in the last decade or so and the connections to spin glasses is object of present attention [11]. Present work is a first application of this tool to determine critical temperatures for the phase transitions in Edwards–Anderson systems.

Possible extensions or applications of this method to other systems are clearly possible and we are presently working on the three-dimensional E–A model. A finite-size scaling analysis is also under way. Different compressors can be used, defined and optimized to better characterize phase transitions. Eventually an appropriate manipulation of data files obtained by analog measurements can also yield critical parameters for stochastic systems.

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