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Effect of the ground-state structure on order parameters in $\pm J$ Ising lattices

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Abstract

The Edwards–Anderson site order parameter, q, or its generalizations have been considered to study the partial spin-glass behavior of $\pm J$ Ising lattices. These parameters vanish if all $2W$ ground states are taken into account, so an ergodic separation must be done in order to emulate nature. Here, we follow a recently proposed criterion to do ergodic separation in spin glasses. The method relies upon: (i) the complete knowledge of the physical properties of the ground level and (ii) a new algorithm to calculate the diluted lattice that remains after removing all bonds that frustrate in any of the ground states. With this new methodology, reproducible values of the order parameters have been obtained. Size effects and tendency towards the thermodynamic limit are established.

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1. Introduction

The two-dimensional Edwards–Anderson (EA) $\pm J$ scheme [1,2] is a model for spin glasses which has been attracting a great deal of interest over the last decades. However, its nature is still not well understood. Complementary to addressing the problem with the help of analytical calculations and computer simulations at finite temperature, it is also possible to obtain a substantial amount of useful information by means of

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exact results for the ground states of the system obtained by alternative methods. Various methods for finding the ground-state structure have been proposed. Some examples are: steepest descent algorithms [2,3], intelligent enumeration using "branch and bound techniques" to avoid high-energy states [3], cluster-exact approximation (iterating clusters of spins) [4], genetic algorithms and ballistic search (sampling of configuration space) [5,6] and recent algorithms [7] combining aspects of previous techniques plus knowledge of properties of configuration space of these systems.

The calculation of physical observables such as the total energy, energy fluctuations, correlation functions, etc. is rather straightforward. However, the calculation of order parameters like the EA site order parameter or the recently reported parameter p [3] requires (i) the exact knowledge of the ground-state level and (ii) to break the ergodicity in some way, separating states from its mirror states. Consequently, order parameters are much difficult to evaluate and it is of interest and of value to inquire how a specific ergodic separation influences the tendency of order parameters towards the thermodynamical limit. In this context, the present paper has four main objectives: (1) to present a strategy to do ergodic separation in spin glasses, which maximizes the order parameters; (2) to make use of a new algorithm to calculate the diluted lattice and parameters p and h [8] (the calculation of the diluted lattice plays a fundamental role in the ergodic separation proposed); (3) to discuss the behavior of the order parameters in a wide range of lattice sizes; and (4) to bring out the advantage of the new algorithm in terms of computer time needed to reach stable results.

2. Basic definitions

In this work, two-dimensional EA $\pm J$ Ising lattices are investigated. They consist of N spins $S_i = \pm 1$, described by the Hamiltonian

$$H = \sum_{\langle i,j \rangle}^{N} J_{ij} S_i S_j \,, \tag{1}$$

where the sum runs over all pairs of nearest neighbors. The spins are placed on a two-dimensional ($d = 2$) square lattice of linear size L and periodic boundary conditions in all directions. Original lattices (samples) are formed by randomly distributing antiferromagnetic (AF) and ferromagnetic (F) bonds in equal concentration. After bonds are allocated they remain fixed at their positions. Then, the $2W$ states forming the ground manifold are reached by calculating all spin configurations minimizing the total energy.

$\pm J$ Ising lattices have been studied for about 3 decades as simple models for spin glasses [1,2]. The original order parameter q to characterize such phase was introduced by Edwards and Anderson and it can be expressed as [1]

$$q = \frac{2}{W(W+1)N} \sum_{\alpha}^{W} \sum_{\beta \geqslant \alpha}^{W} \sum_{i=1}^{N} S_i(\alpha) S_i(\beta) \,, \tag{2}$$

where α and β run over the W states that belong to half of the configuration space (HCS) after breaking ergodicity in a predetermined way. So the case $q = 1.0$ defines

an ideal spin glass, with total site memory, while $q = 0.0$ is a system with no site memory, like a paramagnet.

Later on, other order parameters have been introduced and we would like to consider here the parameter p, which can be defined in the following way [3]:

$$p = \frac{1}{N}\sum_{i=1}^{N}\left\{\left|\sum_{\alpha}^{W} S_i(\alpha)\right| \ \mathrm{div} W\right\}, \tag{3}$$

where $|\cdots|$ means absolute value, while div is an operator meaning integer division, so the expression inside $\{\}$ can take values 0 or 1 only. In a simple way, p can be also obtained by the ratio of the number of spins that never alternate in the half of the ground manifold after ergodic separation over the total number of spins in the lattice.

From the definitions above it follows that states that contribute fully to q also contribute to p. However, states that give partial contribution to q do not contribute anything to p, so $0 \leqslant p \leqslant q \leqslant 1$. Since p is more drastic than q we will restrict from now on to parameter p only.

In all magnetic systems (even a ferromagnet), site order parameters vanish if all ground states are taken into account. So an ergodic separation must be considered. In the case of ideal ferromagnetism there is a singlet ground state, plus its corresponding mirror state (all spins reversed). In such magnet, ergodicity has been broken by nature and we see either the state or the mirror state only. In spin glasses, the application of an external magnetic field to break ergodicity is of no help and there is more than one way of separating states from its mirror states, so ergodicity can be broken in many ways. This point affects significantly results of physical quantities.

3. Results and discussion

The most naive way to do ergodic separation is to fix the position of one spin (i.e., $S_i = +$) on the original lattice, then choosing the W ground states with $S_i = +$ (for the W mirror states $S_i = -$). As an example, we calculate p and q by fixing the position of one spin (in Fig. 1a three possible positions have been selected for illustrative purposes). This methodology provides not reproducible data, since values of order parameters depend strongly on the way the pivot spin is chosen to do ergodic separation. This difficulty can be easily understood by appealing to the concept of "diluted lattice" (DL). The DL associated to an original $\pm J$ Ising lattice is formed by removing all bonds that frustrate at least once through the ground manifold. In Fig. 1b we show the DL corresponding to the original lattice of Fig. 1a. If we designate by B_{DL} the number of bonds in the DL, parameter h can be expressed as $h = B_{\mathrm{DL}}/2N$ [8]. In the case of the lattice illustrated in Fig. 1 it can be easily seen that $h = \frac{75}{128} = 0.5859375$.

In the example, DL is formed by three islands with 60 (39), 11 (9) and 4 (4) bonds (spins), respectively. The spins connected within each island are solidary to each other. Then, if we anchor over the largest island forming the DL (position # 1), the spins belonging to this island remain fixed while the rest modify its state in at least one of the W ground states. Thus, the corresponding value of p can also be calculated by simply evaluating the ratio of the number of spins in the largest unfrustrated domain

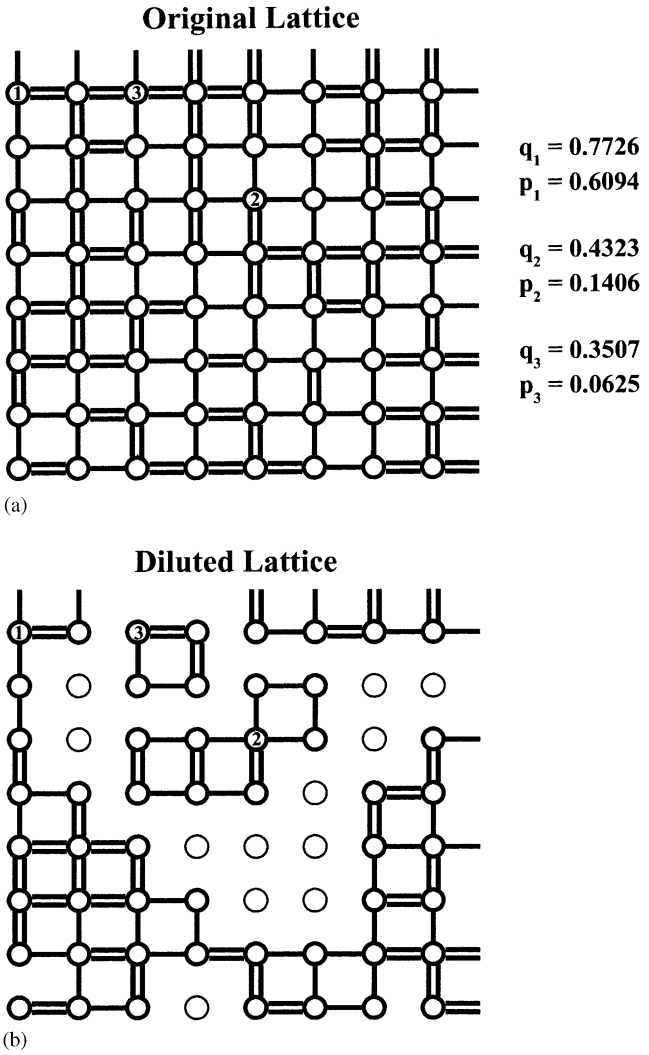

Fig. 1. (a) $\pm J$ square Ising lattice for size 8×8. Single (double) lines represent ferromagnetic (antiferromagnetic) exchange interactions and open circles indicate the position of the spins. The values of q_x and p_x reported in the figure correspond to the values of the order parameters as the ergodic separation is done by fixing the orientation of the spin at site x ($x = 1, 2, 3$). (b) Diluted lattice corresponding to the original lattice (a).

in DL over the total number of spins in the lattice. When this is applied, we get $p = \frac{39}{64} = 0.6094$, which is exactly the maximum value reported for this example. This is equivalent to saying that a considerable energy and time would be needed to overturn a large number of solidary spins. On the other hand, if other ergodic separations are

used (positions # 2,3 in Fig. 1), the existence of such solidary group of spins could be overlooked, thus producing lower values for order parameters, depending on the size of the island we anchor on.

If we consider the largest unfrustrated island only, we get what has been called "maximum" ergodic separation and, consequently, the "maximum" possible value of p.

Therefore, it has been proposed a criterion to do ergodic separation in spin glasses, which takes into consideration the largest cluster in the DL [7]. Then, it is necessary to know the DL of each sample before proceeding to actual calculation of any order parameter. Accordingly, we present next a summary of a new computational algorithm to obtain the DL:

1. An initial state α is chosen at random.
2. By using a steepest descent algorithm, eventually a new state β, belonging to the ground manifold (GM), is obtained.
3. Beginning with state β, a large number of states of the GM is reached by using a single spin flip dynamics at no energy cost. This strategy is continued to generate all interconnected ground states in what is called *invasion* [7]. The lattice that remains after removing all bonds that frustrate in any of the visited states is stored. We called preliminary diluted lattice (PDL) to this set of bonds.
4. A bond, J_{ij}^{*}, belonging to the PDL is chosen at random.
5. A configuration of spins is set at random with the restriction that J_{ij}^{*} remains frustrated in this state.
6. Under these conditions, i.e., with fixed S_i, S_j and $J_{ij}^{*}S_iS_j = 1$, a steepest descend is tried.
   - If GM is reached, J_{ij}^{*} is removed from the PDL, a new *invasion* is invoked and PDL is updated.
   - If GM is not reached, J_{ij}^{*} belongs to the DL.
7. Repeat from point 4, searching for a new bond belonging to the PDL.

This iteration scheme is repeated until eventually the DL is determined. This can be the only possible way of achieving this purpose in the case of large enough lattices where exact calculations are not available.

Fig. 2 shows the tendencies of both h and p as a function of the size N, calculated by using the algorithm described above. Values reported for each size correspond to average value over results for 2000 independent samples generated randomly. Sizes vary from $N = 16$ to 256. Comparison of new data coming from the above algorithm with exact evaluations obtained by direct enumeration of states [8] has been a test for the correctness and accuracy of the new algorithm. This comparison can be done for limited lattice sizes (up to $N = 64$), where exact values of physical quantities are available. For larger sizes we rely exclusively on the new method.

The algorithm proposed above to reach the DL is very efficient and allows us to calculate larger lattice sizes as compared to the capabilities of exact enumeration schemes. Thus, to obtain the DL for 500 samples for $N=36$, it is necessary to run 1075 s the program on a PENTIUM III, 850 MHz using exact calculations based on branch-and-bound algorithm. To obtain the same DL, for the same set of samples using the algorithm

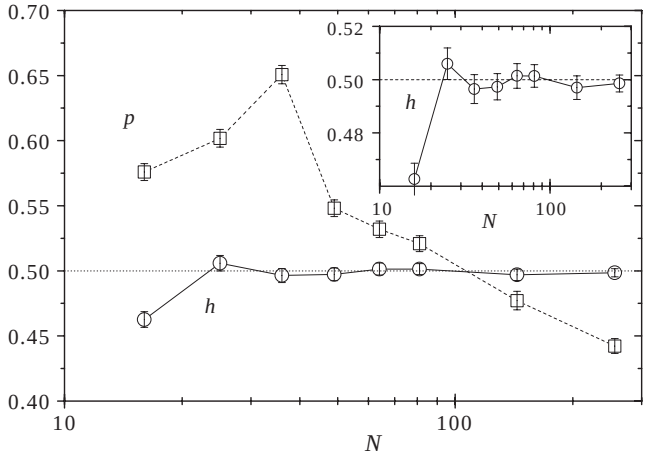

Fig. 2. Parameters h and p as a functions of the size N.

proposed here in the same computer, such time drops to 202 s. This time economy effect is more relevant as size increases.

Finally, as it can be observed from Fig. 2, h remains almost constant, at about 0.50 for lattice sizes ranging between 16 and 121. However, the largest sizes show a smooth decreasing tendency toward the thermodynamic limit. This tendency is better reflected in the behavior of the site order parameter p. With our present computational capabilities, it is not possible to discern whether this result represents a monotonous decrease, or whether its simply a fluctuation.

4. Concluding remarks

Ergodic separation must be done before reporting order parameters to obtain reproducible results. The ergodic separation method called "maximum" has the most clear physical meaning leading to maximum values for p. Such ergodic separation can be easily done once the DL is reached, since then it suffices to anchor on the largest unfrustrated island. To obtain such DL for any sample we propose here an algorithm which proves to be notably more efficient than other previous exact methods. This allows to reach size $N = 256$, where only approximate calculations are possible using "intelligent" enumeration methods. Once the DL is obtained, ergodic separation is possible and calculation of order parameters is easy. Such order parameters do not show a definite tendency toward the thermodynamic limit in the studied range of N. However, rather than attempting a determination of the values of the parameters h and p for $L \to \infty$; the main points of the present paper have been: (1) to emphasize the importance of an adequate ergodic separation in evaluation of order parameter, (2) to establish a criterion for doing the more convenient ergodic separation in order to maximize the numerical values of the order parameters, and (3) to present a new

algorithm which implements the criterion mentioned in (2) in an efficient way. If no attention is paid to ergodic separation, nonreproducible values of order parameters are obtained.

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References

[1] M. Mezard, G. Parisi, M.A. Virasoro, Spin Glass Theory and Beyond, World Scientific, Singapore, 1987.
[2] K. Binder, A.P. Young, Rev. Mod. Phys. 58 (1986) 801.
[3] E.E. Vogel, J. Cartes, S. Contreras, W. Lebrecht, J. Villegas, Phys. Rev. B 49 (1994) 6018.
[4] A.K. Hartmann, Physica A 224 (1996) 480.
[5] A.K. Hartmann, J. Phys. A: Math. Gen. 33 (2000) 657.
[6] K.F. Pál, Physica A 223 (1996) 283.
[7] E.E. Vogel, A.J. Ramirez-Pastor, F. Nieto, Physica A 310 (2002) 384.
[8] E.E. Vogel, S. Contreras, F. Nieto, A.J. Ramirez-Pastor, Physica A 257 (1998) 256.