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# Detailed structure of configuration space and its importance on ergodic separation of $\pm J$ Ising lattices

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## Abstract

A complete and exact characterization of the configuration space of 2-D  $\pm J$  Ising lattices is performed. A new algorithm is introduced here representing advantages for reaching all states for small samples and doing a non-biased sampling of ground states for larger samples. We report efficient procedures to find all ground states grouped in local ensembles of ground states (LEGs) and also a convenient way of storing and comparing states. Properties of such LEGs differ from some approximate descriptions reported in the literature. The onset of lattice size dependence of properties is discussed. Four different ways of performing ergodic separation are used to calculate order parameters. The most significant way of doing ergodic separation requires previous classification of states in LEGs. © 2002 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

The problem of  $\pm J$  Ising lattices simulating spin glasses has been around for many years [1]. In spite of the simplicity of its formulation, serious difficulties arise when trying to achieve, even numerically, a description of all ground states [2,3]. Moreover, the interpretation of some results is subject of controversy and discussion, leaving several open questions [4,5]. Large efforts are put on algorithms attempting to provide

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an approximate description of the configuration space. Some examples are genetic algorithms [6], cluster-exact approximation [7], ballistic search [8], and flat histogram method [9].

Very recently [10], an application of some of these ideas has been done attempting to relate properties of 3-D real lattices to the hierarchical structure of the configuration space by means of sampling of ground states. In the present paper we want to apply a new method to go beyond aiming at a complete description of the configuration space, namely, including *all* ground states. We pay the price of limiting ourselves to square lattices (2-D). The exact description of the ground manifold leads us to the calculation of some known parameters as well as to the introduction of some new parameters whose importance is discussed below. Our results lead to differences with respect to some assumptions usually done with respect to the way ground states are interconnected. We argue that such differences may affect results of physical parameters. We also find that ground states group themselves in a way that allows different ways of performing ergodic separation, leading to ranges of values for any given parameter as it is shown below. In fact, in previous works [11–14] two of such separations were defined leading to different numerical evaluations of magnetic memory associated with spins. These two topology based methods are recovered here from the perspective of the structure of the configuration space. Additionally, we include two new ways of performing ergodic separation to set a lower bound for the range of parameters and also to look at the case of extremely low temperature when the system is trapped in a portion of the configuration space only. This approach based on four different ergodic separations will be applied to two different site-order parameters.

The systems under study consist of square lattices with  $L \times L = N$  spins interacting via nearest neighbor interactions  $J_{ij}$  that can be either ferromagnetic ( $J_{ij} = -J = -1$ ) or antiferromagnetic ( $J_{ij} = J = 1$ ), randomly distributed in equal abundance over fixed positions through the lattice. An example of an  $8 \times 8$  sample is presented in Fig. 1a. Each distribution of interactions is called a sample and we use 500 of them for sizes  $N = 16, 25, 36, 49, 64, 81$ , and 100. Such system is modeled by an Ising Hamiltonian of the form

$$H = \sum_{i < j}^N J_{ij} S_i S_j \quad (1)$$

using periodic boundary conditions. This Hamiltonian is invariant under the simultaneous inversion of all spins ( $S_i \rightarrow -S_i, \forall i$ ), yielding an overall degeneracy factor of 2.

For any given sample we find all possible ground states by two different and independent methods: a version of the well-known exact branch and bound (BB) algorithm for enumerating all low-energy states [11,17] and a new computer algorithm which we call “expansion-fall-invasion-spring” (EFIS) to be briefly presented in Section 2. We begin Section 3 by testing the new numerical method to calculate ground-state energy as a function of size, extrapolating these results toward the thermodynamic limit. Ground states are found in clusters or local ensembles of ground states (LEGs) in such a way that they are connected in pairs by single spin flips at no energy cost. Properties of LEGs are then established reporting new results concerning sizes as well

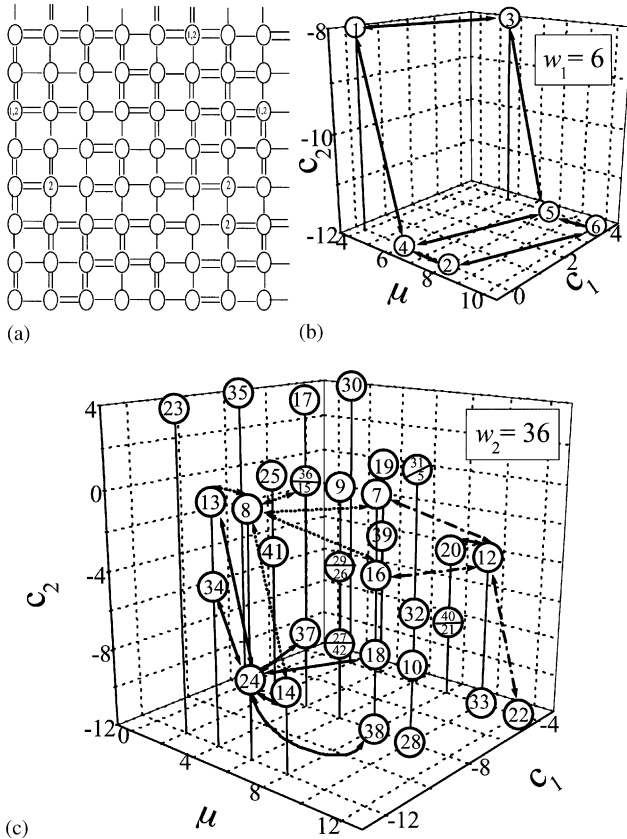


Fig. 1. (a) Sample # 40 from a set of 500 samples  $8 \times 8$ ; ferromagnetic (antiferromagnetic) interactions are indicated by single (double) bars. This sample has 42 ground states (plus 42 mirror states) that can be grouped in two LEGs. (b) Six states belonging to LEG # 1 shown as spheres in the 3-D space defined by magnetization, and the leading two neighbor coordinations. (c) Thirty-six states belonging to LEG # 2 (notice that five spheres represent two different states). LEG # 1 (2) is obtained by alternating spins marked by 1 (2) in the lattice illustrated in (a).

as distances among LEGs. Next we examine the internal structure of LEGs reporting for the first time connectivity among states of the same LEG and the way this novel property scales with size. Finally, we examine four different ways of performing ergodic separation, discussing the implications of this point on the numerical calculation of physical parameters. Section 4 is devoted to conclusions.

## 2. Numerical calculations

Results reported in the next section were obtained by two different methods. On the one side the already mentioned method BB [11,17] and EFIS are used here for

the first time. BB is an exact method based on an “intelligent” way of scanning all low-energy states; we will not give here further descriptions of the method referring the interested reader to the literature. EFIS will be presented here in a general way, avoiding technical computational details to be published elsewhere. The idea is to use results obtained by the exact method to tune EFIS to produce the same results after an appropriate number of iterations.

We next briefly describe the four steps of EFIS algorithm. As we do so, we also describe the way in which physical parameters are calculated. Definitions of new parameters are also included here.

*Expansion:* A *seed state* is randomly generated. Then  $(N - 2)/2$  additional states are generated from the seed state in predetermined ways, so each seed state expands to a total of  $N/2$  expanded states. The expansion algorithm is designed so that the Hamming distances among these expanded states are between  $N/4$  and  $N/2$ , to ensure that such initializations are started far from each other in configuration space. A total of  $n_s$  seed states are prepared so that a total of  $(Nn_s)/2$  initial states are started for each sample. Values for optimal  $n_s$  are size dependent as will be discussed below.

*Fall:* From each initial state a steepest descent procedure is applied minimizing energy by flipping spins sequentially and randomly in turns; when no further minimization is possible, energy is compared with a previously stored minimum energy; eventually a ground energy  $E_g$  (lower energy) is reached and previous false ground states are discarded. On the other hand, if the found energy coincides with  $E_g$ , an efficient comparison procedure is started to see if the state is new, in which case, next step is invoked, otherwise *fall* is initialized with next expanded state. After all these additional initial states are exhausted, a new seed generated by *expansion* is started.

*Invasion:* When a new ground state is reached, all spins are flipped testing for free spins (subject to zero field); when they are found they are marked and counted. Such number represents the *connectivity*  $C$  of that state, namely, the number of ground states that can be reached by a single spin flip at no energy cost. *Each* new ground state is subject to the same procedure in such a way that *all* ground states interconnected by single spin flips are generated. Such set of interconnected ground states has been called “valley” [18], “funnel or cluster” [8,10] and “local ensemble of ground states (LEG)” [19]. We will stick to the last denomination. For each state of a LEG we measure connectivity  $C$ , ground energy per bond  $\varepsilon_g = E_g/(2N)$ , magnetization per site ( $\mu = \sum_i^N S_i/N$ ), site order parameters  $q$  and  $p$  (defined below), nearest-neighbor correlation  $c_1$ , and second-nearest-neighbor correlation  $c_2$  [11].

*Spring:* Once a LEG is exhausted, we go over each of its  $w$  states simultaneously flipping sets of spins according to predetermined patterns. If after the simultaneous inversion of the set of spins the same  $E_g$  is obtained, a different LEG has been reached (if new energy is lower than  $E_g$  all counters are reset, false ground states erased and the process starts all over). Such process of changing to another ground state by flipping several spins at a time is a jump or *spring* in the configuration space. Occasionally, such spring leads to landing on a LEG which has not been characterized yet. If that is so, such state is stored. Once *spring* is over, *invasion* is invoked for each of these stored states. Procedure *spring* is invoked from each new LEG until no new LEGs are generated. The number of spins to be flipped in each jump and their geometrical

distribution are determined by the preferred shapes and sizes present in the diluted lattice obtained after removing all bonds that frustrate in any ground state [14,19,20]. Special cellular automata are prepared to handle this process in a fast and efficient way. For results reported below, we considered one shape for cellular automata of 2–5 spins and two shapes for cellular automata of 6–8 spins in all possible orientations. Once *spring* is fully exploited, a new initial state is considered until reaching  $n_s$  runs.

$n_s$  is increased until all results obtained by EFIS exactly agree with results obtained by BB. This procedure was done up to  $N \leq 64$ . Beyond this point computer times needed by BB are extremely large. However, an extrapolation was done to estimate the appropriate values of  $n_s$  for  $N=81$  and 100. In any case, we did more initializations than indicated by such estimates to make sure that all true ground states are reported. Thus, for  $N=100$ , we used  $n_s = 10^6$ . Beyond this point, storage capabilities for LEGs and computer time needed grow beyond our present computer capabilities (cluster of Pentium III).

### 3. Results and discussion

Before going into the properties of the ground manifold (main aim of this paper), let us test the merits of EFIS by measuring  $\varepsilon_g(N)$  and comparing these results with those obtained by BB and also with the results available in the literature including scaling toward thermodynamic limit ( $N \rightarrow \infty$ ). Circles in Fig. 2 represent values for  $\langle \varepsilon_g(N) \rangle$  obtained by EFIS; they fully coincide with the results obtained by BB up to  $N=64$ . So EFIS is able to give exact results for small systems using far less time than BB. (Technical points concerning algorithm structure and performance will not be discussed here.)

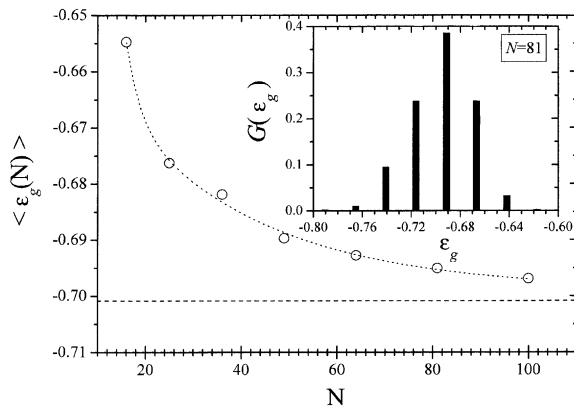


Fig. 2. Average ground state energy per bond  $\langle \varepsilon_g(N) \rangle$  obtained by EFIS. Curve with short dashes corresponds to the exponential fit of these points as discussed in the text. Line with long dashes represents the asymptotic value for the exponential fit in good agreement with Ref. [18]. The inset illustrates the relative distribution of energies among the set of samples for  $N=81$ .

Short-dashed curve in Fig. 2 represents an exponential fit for the seven points calculated by EFIS, by means of the expression

$$\varepsilon_g(N) = -0.700845 + 3.52606 \exp(-N/2.88887). \quad (2)$$

The long-dashed horizontal line corresponds to the asymptotic value of previous expression as  $N \rightarrow \infty$ . Namely,  $\varepsilon_g(\infty) \approx -0.701$ . It is interesting to compare this value with the recently reported extrapolation yielding  $-0.70097$  obtained by means of faster computers applied to larger lattices [21]. This agreement, including points  $N = 81$  and  $100$  not previously validated by BB, indicate that EFIS leads to reliable extrapolations for larger systems.

However, ground manifold energy is the less-sensitive parameter since it is enough to hit just one (any) ground state per sample to build a curve like Fig. 2. Calculation of other physical parameters requires the knowledge and storage of *all* ground states. So we now turn our attention to the entire ground manifold.

All ground states obtained by simultaneously reversing all spins in each ground state of a LEG form its *mirror* LEG. The number of ground states forming the  $\ell$ th LEG is the size of the LEG and will be denoted by  $w_\ell$ . Let us denote the number of pairs of mirror LEGs by  $v$ . Then, the total degeneracy of such disjoint ground manifold can be written as

$$2W = 2 \sum_{\ell=1}^v w_\ell. \quad (3)$$

This characterization is done for each sample. Thus, for the particular sample illustrated in Fig. 1a we found 2 pairs of LEGs ( $v = 2$ ). Fig. 1b illustrates the first LEG, with  $w_1 = 6$ , states are represented by spheres; connections among them are indicated by lines. Fig. 1c shows LEG #2, with  $w_2 = 36$  and a few connections among states; 16 states have  $C = 4$  (such as state 12), 16 states have  $C = 5$  (such as state 8), and four states have  $C = 6$  (such as state 24). Notice that states are spread in a 3-D representation using  $\mu$ ,  $c_1$ , and  $c_2$  as axes. We developed an efficient way of comparing states saving considerable computer time when looking for new ground states; the actual comparison of individual spins is left for those few cases where states coincide in their “coordinates”, as shown in Fig. 1c where five pairs of states share coordinates.

By using EFIS we calculated  $\langle w(N) \rangle$ , the average size of a LEG over all LEGs in the 500 samples for size  $N$ . These results match exactly those obtained by BB up to  $N = 64$ . Fig. 3 shows that  $\langle w \rangle$  grows exponentially with  $N$ , which is an expected result. Sizes of LEGs follow a distribution  $F(w)$  which is far from trivial as shown in the upper inset, where sizes that are multiples of four and three dominate. We also measured  $D$ , the *distance* between pairs of LEGs defined as the minimum number of spins to be overturned to connect any state of the first LEG to any state of the second LEG. In the lower inset of Fig. 3, we present normalized abundance of distances  $f(D)$  after considering all possible pairs of LEGs through 500 samples of all sizes reported here; this result is new and has interesting implications for EFIS. In fact, this backs the strategy used in *spring* where particular combination of spins is overturned to attempt jumping to a neighboring LEG. Very clearly some distances are more common than

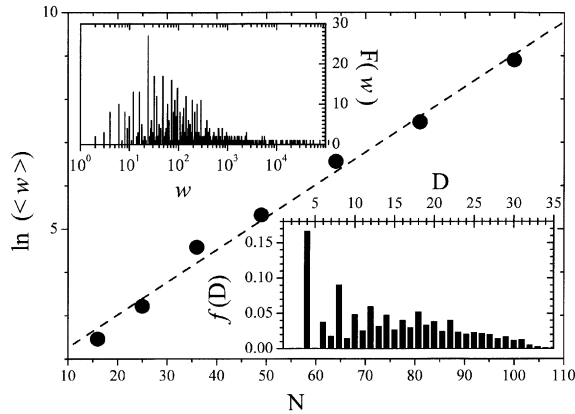


Fig. 3. Average size of LEGs (through logarithmic function) as function of lattice size  $N$ ; dashed straight line justifies an exponential growth of  $\langle w(N) \rangle$ . Upper inset shows the spectral distribution of LEGs ( $N = 81$ ). Lower inset present the distribution of distances among LEGs ( $N = 81$ ).

others. Several abundant distances coincide with sizes for cellular automata included in the *spring* process. Although illustrated here for the case  $N = 81$ , the general fashion of distributions shown in the insets is the same for all sizes.

We also investigated  $\langle v(N) \rangle$  (not shown). It is found that  $\langle v \rangle$  grows with  $N$  in a less pronounced way than  $\langle w \rangle$  as shown in Fig. 3. Further investigation increasing  $N$  is needed to establish whether such growing can be better explained by a weak exponential or a power law. For the time being, we can say that the exponential growth of the total degeneracy  $W$  is mainly due to the exponential growth of LEGs sizes. This is very important since computer times could be lowered substantially if effort is concentrated in finding the first state of a LEG followed by the generation of all remaining states by means of *invasion* or any other similar deterministic algorithm.

An important new result reported here is presented in Fig. 4 where normalized distributions of connectivities  $g(C)$  are plotted for different  $N$  values. To build this graphic every single state of all LEGs has been considered exhausting all possible connections. Several comments are in order. First, for each  $N$  the distribution of connectivities follows a Gaussian as represented by dashed lines. Second, size effects are noticed for  $N \leq 25$ . Third, the first momentum (average) of  $g(C)$  follows a linear behavior with  $N$  as shown in the inset. Fourth, width of the Gaussian grows initially with size with a prompt tendency to stability. Previous properties are very important to consider when sampling states of a LEG. If this is done by just “visiting” states [10], it is inevitable that states with larger connectivity will appear more often than those poorly connected. One immediate effect of such biased sampling can be the underestimation of  $w$ . From a thermodynamic point of view, all interconnected degenerate states are equivalent; highly connected states are visited more times but they are also exited the same number of times thus establishing equilibrium. Poorly connected states cannot be ignored on the basis that are less visited; once the system reaches one of them, it is likely to remain in that state longer than in the more connected states.

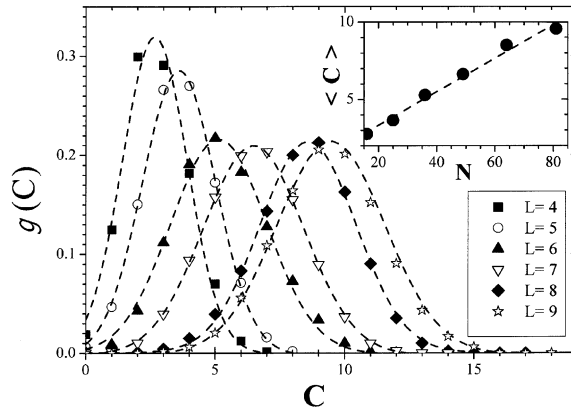


Fig. 4. Distribution of connectivities among states of all LEGs for each lattice size  $N$ . Dashed lines represent the best Gaussian fit for each distribution. Inset shows the linear increase of  $\langle C \rangle$  with  $N$ .

EFIS produces an interesting byproduct: it is enough to store one ground state per LEG after solving for each sample in a first run. To calculate properties and parameters, all states of each LEG may be generated by means of *invasion* in little time.

Once all ground states are known physical properties can be calculated. However, as we will prove, results are not unique and depend on the way ergodic separation is done. We concentrate here on zero-temperature order parameters  $q$  [22] and  $p$  [11,14], which are defined as

$$q = \frac{2}{W(W+1)N} \sum_{\alpha} \sum_{\beta \geq \alpha} \sum_{i=1}^N S_i(\alpha) S_i(\beta), \tag{4}$$

$$p = \frac{1}{N} \sum_{i=1}^N \left| \sum_{\alpha} S_i(\alpha) \right| \mathbf{div} W, \tag{5}$$

where  $\alpha$  and  $\beta$  are two ground states that are connected according to the ergodic separation done on the configuration space;  $\mathbf{div}$  is the integer division operator. Edwards–Anderson parameter  $q$  ponders the orientation of each spin through the  $W$  ground states of half the configuration space. On the other hand, parameter  $p$  measures the fraction of spins that never flip as going over the same  $W$  ground states. Notice that  $p \leq q$ .

Any complete ergodic separation considers  $W$  ground states formed by leaving  $v$  LEGs on half of the configuration space used for further calculations. Such process of forming a basin of  $W$  states can be done in  $2^v$  ways, leading to similar number of calculations for  $p, q$  and any other physical parameters, thus leading to ranges of values for each of them. Large differences may arise depending on whether a LEG or its mirror are left in the basin. We consider here three complete ergodic separations and one incomplete one. They are selected according to the following criteria. *Random* is the simplest case which happens to come out naturally if no thought is given to



the importance of ergodic separation. *Maximum* is the method we consider as truly representative of the physical properties of the system and also is the upper bound for numerical values of parameters. *Minimum* is the less physical ergodic separation but it is included here since values calculated in this way represent the lower bound for parameters. *Frozen* is an incomplete method representing the situation when the system is confined to a portion of the configuration space at extremely low temperatures. We present now how these four methods are technically carried out.

For convenience, we begin by sorting pair of LEGs (LEG and mirror LEG) according to size from larger to smaller; if two or more pairs of LEGs share the same size, an arbitrary order is established among them. First step is to decide whether the largest LEG or its mirror LEG remains in the basin; this decision is arbitrary and the results do not depend on it in any way. One of them is kept while the other is discarded. From this point on ergodic methods differ from each other as we describe next.

*Random*: Second pair is considered and either LEG or mirror LEG is left in the basin in a completely random way. The same procedure is repeated until the  $v$ th pair of LEGs is reached. This procedure is not reproducible since there is no correlation among LEGs left in the basin.

*Maximum*: Distances between each of the two LEGs forming the second pair and the first LEG in the basin is measured. The one with the shortest distance is left in the basin while the other is discarded. This process is continued through all remaining pairs of LEGs. This procedure is reproducible. Moreover, it is quite physical since the basin is formed by the largest LEG plus neighboring smaller LEGs.

*Minimum*: Just the opposite to previous one. LEG with the largest distance to the first LEG are kept in the basin. Although reproducible, it is basically no physical since large number of spins must be simultaneously overturned when scanning the basin. We include it here to set lower bounds to calculation of parameters as discussed above.

*Frozen*: It is an incomplete ergodic separation that considers the first (larger) LEG only. All other  $2(v - 1)$  pairs of LEGs are discarded. This ergodic separation can be very useful at zero temperature, when the system cannot abandon the LEG where it sits. This can be any LEG, of course, but when we consider the largest one we obtain the least possible value for a parameter as the limit of zero temperature is approached.

Fig. 5 shows size dependence for  $\langle p \rangle$  and  $\langle q \rangle$  according to the four ergodic separations where averages are taken over the set of 500 samples for each  $N$ . Large differences are found depending on the way ergodic separation is performed. Moreover, general tendencies point to different interpretations. Thus, if *frozen* separation is performed both  $p$  and  $q$  tend to increase as size grows, speaking of a group of solidary spins, which is close to the droplet-scaling picture [16]. *Maximum* separation tends to give size-independent values for both parameters. On the other hand, if *random* or *minimum* separation are used, both  $p$  and  $q$  tend to diminish steadily with size, speaking of almost free spins all overturning if enough time is allowed, thus favoring nil site order parameters in the thermodynamic limit, which is close to the replica-symmetry-breaking mean-field approach model [15].

Next we review the way two separations based on the real lattice are recovered from the point of view of the configuration space developed here. Let us concentrate first in

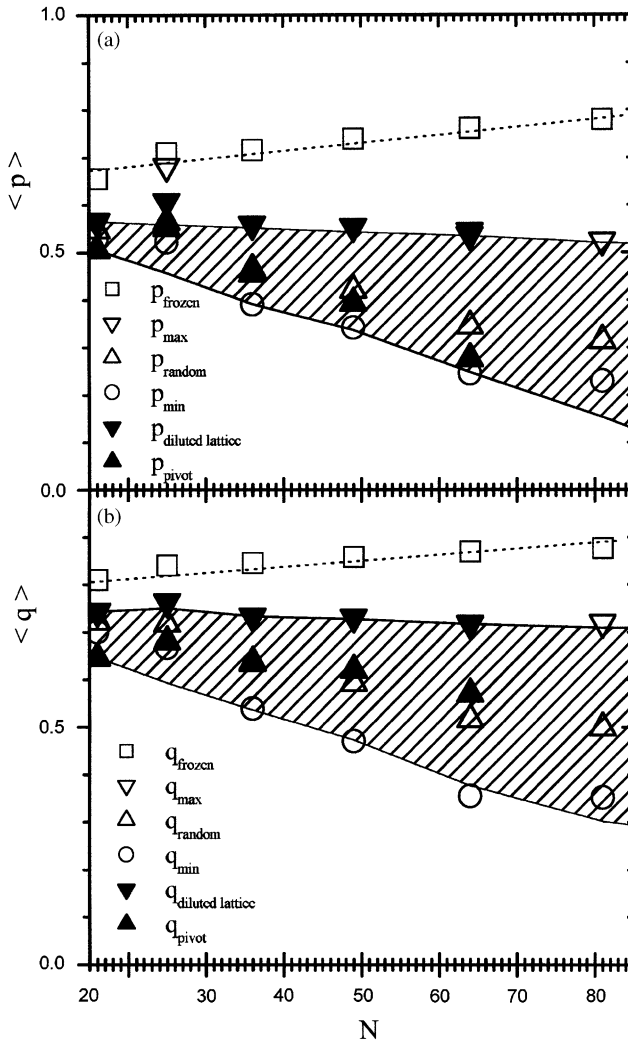


Fig. 5. Lattice size dependence of site order parameters  $p$  (a) and  $q$  (b) calculated after six different ways of performing ergodic separation. Four of these methods, based on properties of the configuration space, are discussed in the text. Results for two other methods, based on topological properties of the lattice, are taken from the literature (Ref. [14]). The dashed area corresponds to the possible values that each parameter can take depending on the way total ergodic separation is performed (limiting lines are only to guide the eye). “Maximum” and “minimum” act as limits for the allowed range; any other ergodic separations (like “random” or “pivot” for instance) lay inside the range. Partial ergodic separation “frozen” is notoriously out of such range since it does not include all LEGs in its formulation. Results by “maximum” and “diluted lattice” overlap completely.

maximum ergodic separation, which it turns out to be equivalent to a previous ergodic separation based on the diluted lattice (the lattice left after removing all frustrated interactions after scanning all ground states) [12–14]. The topological ergodic separation considered all  $W$  states that leave frozen spins on the largest island in the diluted lattice.

The other  $W$  states are obtained upon simultaneously flipping all spins on the largest island of the diluted lattice. Values for parameters obtained by these two methods (one based on the real lattice while the other works in the configuration space) agree sample to sample. This equivalence between maximum and previous topological method speaks of the true physical grounds of this ergodic separation. In Fig. 5 such identical results overlap completely.

If no attention is paid to the way ergodic separation is performed, results are likely to agree in the long run with those given by random separation. One possible way of doing this is that we look for a spin with all four surrounding bonds satisfied in all ground states; such strongly attached spin acts as a pivot [11,14]. Then  $W$  ground states are obtained with this Ising spin pointing up while the other  $W$  ground states correspond to states with this spin pointing down. If by chance such strongly attached spin happens to belong to the largest unfrustrated island we obtain the same value as in maximum. However, such strongly attached spin can also occur at smaller islands in the diluted lattice in which case smaller values for the parameters are reached. When an average over a large number of samples is considered, results obtained by this method are similar to those given by random separation. It is very likely that some of the reported values in the literature correspond to this method in one way or another [11].

The dashed sectors in Fig. 5 illustrate the range of values that can be expected for different ergodic separations. Namely, maximum and minimum lead to upper and lower bounds for any calculated parameter, respectively. Clearly, tendencies toward thermodynamic limit are also affected by this growing range as  $N \rightarrow \infty$ . However, if we stick to maximum only as the most representative way of doing ergodic separation from a physical point of view, almost constant values for order parameters are obtained as size grows.

#### 4. Conclusions

The ground manifold of configuration space can be understood as a collection of  $W$  (plus  $W$ ) ground states grouped in  $v$  LEGs. Sizes  $w$  of such LEGs follow extended irregular distributions presenting one dominant or largest LEG for each sample (Fig. 3). As lattice size  $N$  increases,  $\langle w \rangle$  grows exponentially. The number of pairs of LEGs  $v$  also grows with  $N$ ; larger samples should be solved before deciding whether this growth is exponential or just polynomial.

Distances among LEGs prefer certain number of spins in particular geometric distributions. This encourages the development of algorithms (such as EFIS) which can connect most of the LEGs of a system by overturning predetermined patterns of spins in the way defined for stage *spring* above.

EFIS was able to reproduce the configuration space found by exact method BB up to  $N = 64$ . From there on a reliable way of extrapolating for the necessary number of runs  $n_s$  was found. In this way lattices of larger sizes can be tackled much faster than using BB.

Within a LEG, states present different values for connectivity  $C$ . The distribution of  $C$  can be fitted according to Gaussian curves whose centers increase linearly with lattice size  $N$  (Fig. 4). Several important consequences arise from this fact. First, connectivity tend to increase linearly with lattice size. Second, size effects in the shape of the distribution seem to disappear for  $N \geq 36$ . Third, the distribution does not spread significantly; independent of lattice size there are about 12 relevant  $C$  values approximately described by a Gaussian distribution. Fourth, care must be taken in the way a LEG is sampled since highly connected states can show more than less connected states; a biased sampling can lead to wrong description of configuration space.

The complete knowledge of the configuration space achieved here allows different ergodic separations. If no attention is paid to the structure of the ground manifold, equivalent to *random* ergodic separation, site-order parameters tends to diminish with size, so no order parameter should prevail in the thermodynamic limit. This is even more so if *minimum* ergodic separation is invoked; this is rather unphysical. If physical considerations are taken into account to decide ergodic separation, like in *maximum* separation, site order parameters show a more stable tendency with size. However, larger lattice sizes would be needed to decide whether this is a property that can still hold toward the thermodynamic limit. Alternatively, if the system is getting trapped in one LEG as temperature approaches zero, strong and growing site order parameters are found; this is so even if the largest LEG is invoked to do this *frozen* ergodic separation.

The complete knowledge of the configuration space is needed to perform proper ergodic separation. Then, each sample has to be solved twice: the first instance is for getting all LEGs and doing ergodic separation; the second time to go over states to actually calculate properties. If this is not done, results for any sample could not be even reproducible, since values of parameters depend strongly on the way ergodic separation is performed as presented in Fig. 5. From physical consideration *maximum* ergodic separation should be done at any temperature, eventually turning to *frozen* ergodic separation for very low temperatures.

Finally, we want to stress that EFIS was fully tested as an exact algorithm up to  $N = 64$ . A reliable way of extrapolating this algorithm to get an accurate description of the configuration space of larger systems was indicated; this was applied to the cases of  $N = 81$  and 100. By means of faster computers further extrapolations should be possible. In any case, EFIS can also be used as an unbiased approximate method to explore configuration space.

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