Percolation in correlated and non-correlated diluted triangular Ising lattices

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Triangular lattices with N spins interacting by means of $\pm J$ bonds are described by an Ising Hamiltonian. Equal number and equal strength are assumed for ferromagnetic and antiferromagnetic interactions. The low-energy portion of the configuration space is completely scanned. It is found that the ground manifold is usually split into several ensembles of connected ground states in the configuration space. Once they are known several physical properties can be calculated: order parameters, correlations, magnetization. Frustration arises as a competition of randomly distributed interactions. When frustrated bonds are removed, a diluted lattice is defined. Occupied sites in the diluted lattice are regions free of frustration that happen to prefer certain sizes and shapes. Some of these regions get large enough to percolate. We will perform a statistical analysis of the above mentioned properties, using 7000 randomly generated samples for the case of $N = 36$.

Keywords: Ising lattices; frustration; order parameters

Se considera una red triangular de N espines, con interacciones mixtas $\pm J$ y aleatoriamente distribuidas a primeros vecinos. De las $3N$ interacciones, la mitad son ferromagnéticas y la otra mitad antiferromagnéticas, todas con igual magnitud. Mediante simulación computacional y usando algoritmos que barren completamente la porción de baja energía del espacio de Hilbert, se encuentran todos los posibles estados fundamentales. Con ello se calculan parámetros de orden, correlaciones y magnetización. La frustración aparece por la alta competencia de interacciones mixtas aleatorias. Si los enlaces frustrados son retirados de la red, surge la red diluida, en la que no hay ningún tipo de frustración. Se encuentra que la red diluida presenta regiones o dominios libres de frustración, con formas y tamaños preferidos. Más aún, estas regiones muestran un alto grado de percolación. El presente trabajo se basa en un estudio estadístico sobre 7000 muestras generadas al azar para el tamaño $N = 36$.

Descriptores: Red de Ising; frustración; parámetros de orden

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1. Theory and methodology

Disordered systems presenting short range order have been subject of several studies in the last years. [1–3] We consider here an Ising Hamiltonian, [4] where $\pm J$ competing interactions are randomly distributed through a triangular lattice of size N, given by the number of spin sites [5, 6]

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

The admixture of ferromagnetic ($J_{ij} = -J = -1$) and antiferromagnetic ($J_{ij} = +J = +1$) interactions can lead to order-disorder transitions. Another interesting feature of these systems is the presence of frustration with all its implications [7, 8].

In the present paper we restrict ourselves to equal concentration of ferromagnetic and antiferromagnetic interactions for lattices of $N = 6 \times 6$ spins using periodic boundary conditions. 7000 samples were randomly prepared beforehand; bonds are not altered at all for the rest of the calculations.

Computer algorithms were prepared so all the $2W$ ground states can be found. In fact it is enough to work with half of the configuration space due to the inversion symmetry of the Hamiltonian. All of the properties of each ground state are found. In the present paper we emphasize the results dealing with frustration in the lattice, looking at the regions without frustration that arise after removing all bonds that frustrate in any of the W ground states. It turns out that size and shape of unfrustrated regions are not trivial. Moreover, about 80% of the lattices diluted by frustration percolate due to unfrustrated regions that get large enough. As a comparison only 70% of uncorrelated lattices of similar bond content percolate.

In Fig. 1, we illustrate all these concepts. Frustrated plaquettes are marked by black dots; they are paired by means of frustration segments that go over frustrated bonds as can be seen for a particular ground state in Fig. 1a. Periodic boundary conditions hold.

The diluted lattice is formed by removing all bonds that frustrate in at least one of the W ground states. In Fig. 1b we illustrate the diluted lattice corresponding to the original lattice given in Fig. 1a. The ratio between the number of bonds in the diluted lattice and the number of bonds in the original lattice is called the fractional content of bonds in the diluted lattice and it is denoted by h_g. In this illustration we also appreciate that unfrustrated bond cluster in regions of different sizes and shapes.

The largest region of unfrustrated bonds is isolated in Fig. 1c. The ratio between the number of bonds in the largest region and the total number of bonds in the original lattice is

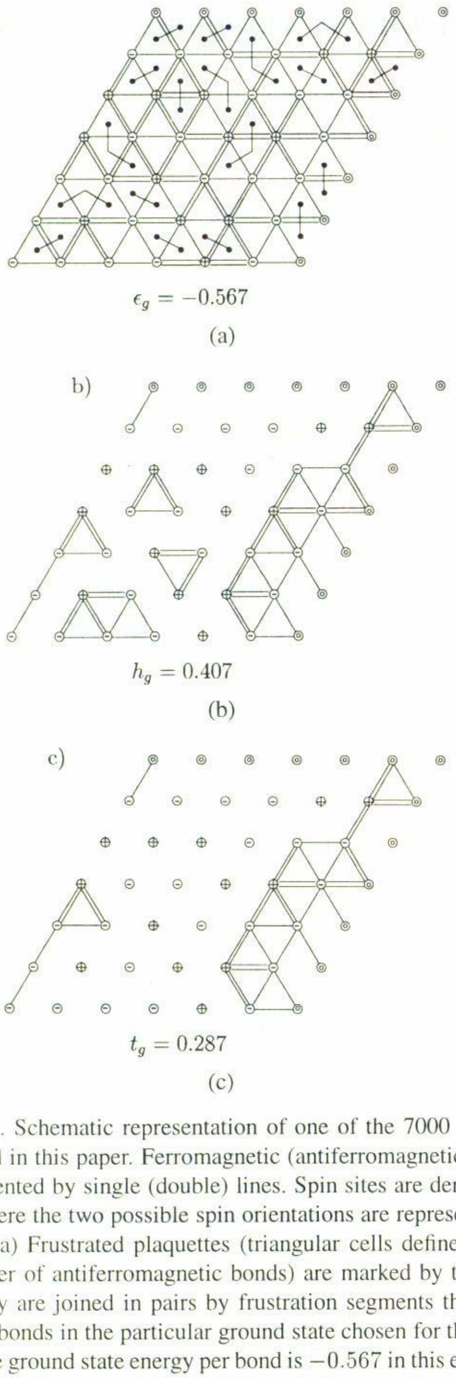


FIGURE 1. Schematic representation of one of the 7000 samples considered in this paper. Ferromagnetic (antiferromagnetic) bonds are represented by single (double) lines. Spin sites are denoted by circles where the two possible spin orientations are represented by $\pm$ signs. (a) Frustrated plaquettes (triangular cells defined by an odd number of antiferromagnetic bonds) are marked by the symbol $\bullet$; they are joined in pairs by frustration segments that cross frustrated bonds in the particular ground state chosen for this illustration; the ground state energy per bond is -0.567 in this example. (b) Diluted lattice generated from lattice a) after removing all bonds that frustrate in any of the ground states; regions of different sizes and shapes arise naturally in the diluted lattice; the fractional content of bonds in this diluted lattice is 0.407. (c) Largest unfrustrated region found in the diluted lattice; in this example percolation is present; the fractional bond content of the largest region is 0.287 in this case.

the fractional content of bonds corresponding to the largest region and it is given the symbol t_g. From this example we can see that the largest island is built from unfrustrated triangular plaquettes as basic unit. Moreover we see that in this example the largest region percolates.

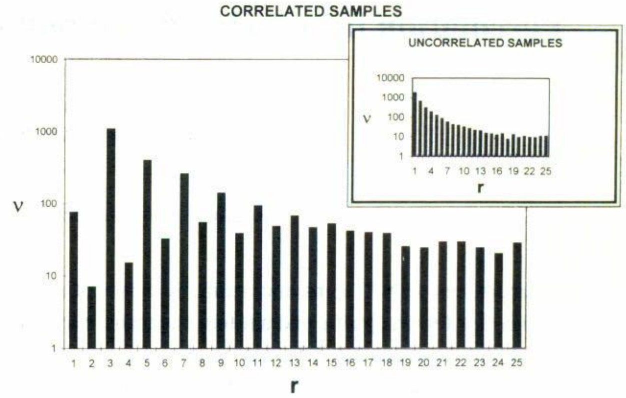


FIGURE 2. Spectral distribution of regions in the diluted lattice according to their size r. The log scale shows that regions of size 3 are by far the most abundant. Such distribution is very peculiar and completely different from the monotonic behavior presented by uncorrelated diluted lattices generated at random as shown in the inset.

For comparison we prepared random or uncorrelated diluted lattices by just assigning the fractional content of bonds in a completely random way. In fact, 200 lattices for each of the following fractional contents were prepared randomly: 1/108 (one bond in the diluted lattice over 108 in the saturated lattice), 2/108, 3/108, ... , up to 108/108. For each of these 21 600 samples we looked for sizes and shapes of regions of connected bonds; special care was paid to establish wether the largest region percolates.

2. Results

Let us define the size r of a region of bonds by the number of connected bonds that form it. In Fig. 2, we show the spectral distribution of regions according to their size r obtained with 2000 samples. Results for diluted correlated lattices are presented in the main body of the figure, while results for randomly generated (uncorrelated) lattices are shown in the inset. The modulation observed for correlated lattices (sizes with odd number of bonds are more abundant) is absent for random lattices of the same bond content. Clearly dilution obtained by eliminating frustration leave some kind of correlation among the remaining bonds.

Regions of size 3 are the most abundant. We did a separate investigation for this size finding that the absolutely dominant shape for this size is a triangle formed by an unfrustrated plaquette. In the case of uncorrelated lattices, the 12 possible shapes for size 3 are present in the numerical simulations in very good agreement with analytic studies based on combinatorial theory. Back to correlated lattices, we observe that small unfrustrated regions with even number of bonds are very scarce. At $r = 15$ difference between even and odd sizes disappears and abundances are spread to quite large sizes.

The most relevant shapes for unfrustrated regions are presented in Fig. 3 using the same 2000 samples employed in

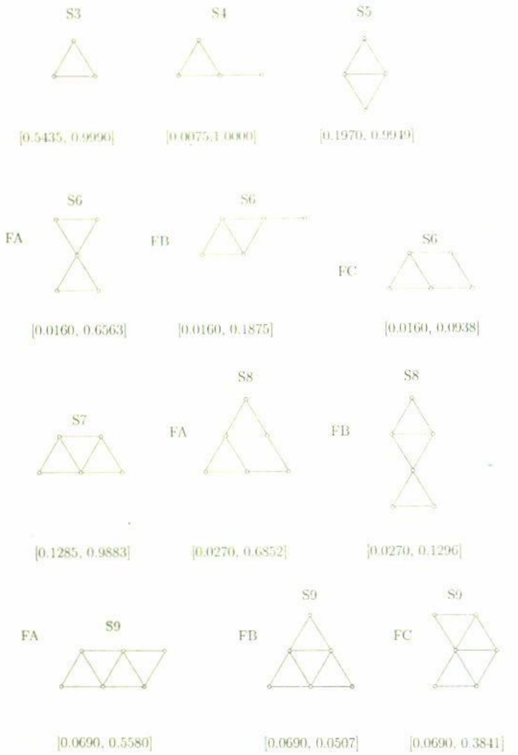


FIGURE 3. Shape analysis for sizes $3 \leq r \leq 9$. Sr represents a relevant shape for size r; when there are several relevant shapes for a given size, they are denoted by FA, FB, $\ldots$ in a sequential order. The brackets contain two numbers consecutive numbers in the form $[N1, N2]$: $N1$ is the relative abundance of this size within lattices $N = 36$, while $N2$ is the relative abundance of that particular shape within all regions of that size.

Fig. 2. Symbol Sr refers to size r. In brackets we give two numbers in the form $[X, Y]$: X represents the probability of finding a region of that size (any shape) for lattices 6×6; Y represents the probability of finding that particular shape within the universe of all the regions of that size. Only the most important shapes are reported. It is also found that for correlated lattices large regions are fundamentally formed using the region of size 3 as building block.

Reasons behind these preferred sizes and shapes are topological. The smallest circuit of bonds is a triangle that is named plaquette. A plaquette formed by an odd number of AF bonds is curved or frustrated since it cannot satisfy all fields around it. Frustrated bonds correspond to those that are crossed over when joining pairs of frustrated plaquettes. So in a neighborhood where there are curved plaquettes bonds are likely to frustrate and they will not show up in the diluted lattice. On the other hand, in a neighborhood where there are plenty of flat plaquettes there is a high probability for the absence of frustration, leaving an unfrustrated region. Then unfrustrated plaquettes are a necessary condition for the building blocks of large unfrustrated region. However, it is not a sufficient condition, since a flat plaquette can be crossed over completely to connect two neighboring curved plaquettes over it as seen in Fig. 1a.

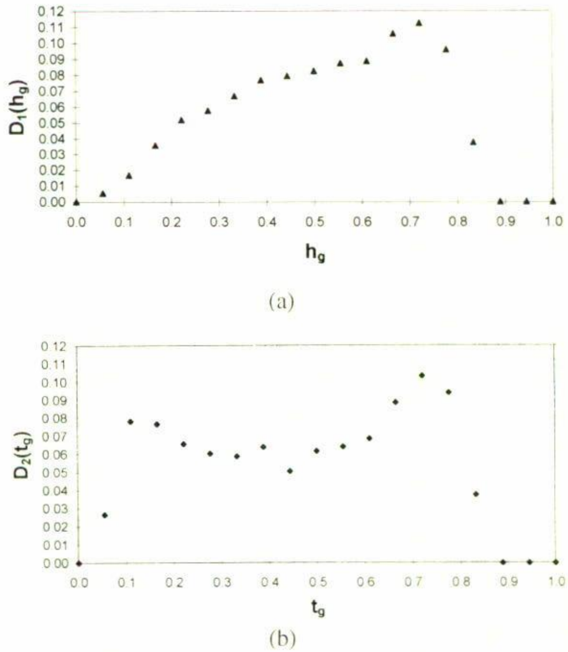


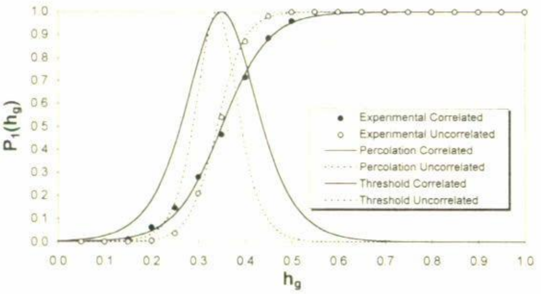
FIGURE 4. Distribution functions for the percolation parameters as produced by the samples with the only constraint of having equal number of ferromagnetic and antiferromagnetic bonds. (a) Distribution D_1 corresponding to the number of samples for each interval in the h_g range. The distribution is clearly asymmetric, maximizing at about 0.72. (b) Distribution D_2 giving the number of samples with the largest region for each channel defined in the t_g axis. Such distribution suggests a bimodal.

Now we turn our attention to the percolation properties of the diluted lattice. We have two choices for the percolation parameter: h_g and t_g already defined above. $\pm J$ Ising lattices with equal amount of F and AF bonds produce a great variety of samples with a broad distribution for these parameters. In Fig. 4a we present the distribution $D_1(h_g)$ of values of h_g while in Fig. 4b we present the distribution $D_2(t_g)$ for values of t_g. In both cases a total of 7000 triangular samples of size 6×6 were used.

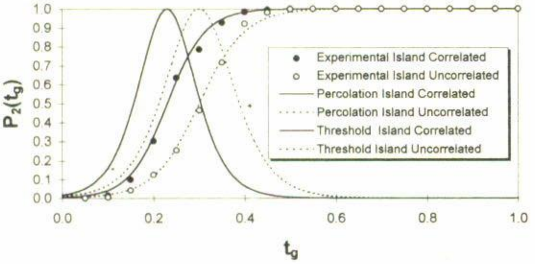
The natural distribution of values for h_g is very similar to the corresponding distribution for square lattices [9]. We have enough samples to perform statistics within each channel for h_g values in the range $[0.15, 0.85]$. So we will use this natural distribution to construct the percolation curve.

On the other hand, the distribution curve D_2 for values of t_g shows a different behavior: it is broader than D_1 especially for low values of t_g; it is flatter than D_1 but showing two maxima one at about 0.1 and the other at about 0.75. The most important point is that for all values of t_g in the interval $[0.05, 0.85]$ there are many samples so a percolation probability can be calculated.

For comparison purposes we prepared random diluted lattices with previously defined bond content h_g. Then, we did a flat distribution in the range $[0.0, 1.0]$. This does not make a substantial difference in the results since the statistics are normalized within each channel created for the values of the



(a)



(b)

FIGURE 5. Percolation analysis. (a) Percolation is studied in terms of the fractional bond content in the diluted lattice h_g. (b) Percolation is now studied as function of the bond content if the largest unfrustrated region t_g. Symbols are defined in the corresponding insets. In both cases we report the results of the numerical experiments (circles), the interpolated percolation curve and the first derivative of previous curve to find the inflection point that can be associated to the percolation threshold.

percolation variable. For these uncorrelated diluted lattices we also isolated the largest region per sample to obtain the t_g values for each sample.

In Fig. 5a we show 2 percolation curves $P_1(h_g)$ and their corresponding first derivatives. Filled circles represent the percolation probability for correlated lattices as a function of h_g; the solid line is a fit to these points. Open circles represent the percolation probability for uncorrelated lattices; the dashed line is a fit to these points. The solid line maximizing at about 0.34 is the first derivative of the former, while the similar dashed curve maximizing at about 0.32 is the first derivative of the latter. Percolation threshold is broader for correlated diluted lattices then the threshold for randomly generated lattices of the same bond content. The result for uncorrelated lattices coincides with the expected value in the thermodynamic limit [10].

In Fig. 5b we do the same analysis for the $P_2(t_g)$, the percolation curves in terms of the largest region. Now several differences arise. First, the percolation threshold is obtained for lower values of t_g for both lattices. Second, the percolation threshold is lower for correlated lattices (0.23) as compared to uncorrelated lattices (0.30). Third, the transition for correlated lattices is sharper in terms of t_g as compared to the same transition for uncorrelated lattices.

3. Concluding remarks

We conclude that triangular diluted lattices formed after removing all bond frustration exhibit regions of preferred size and shape due to the original topology present in the lattice. Such effect is absent in uncorrelated lattices. At present we are obtaining some initial analytic calculations based on topology that explain this phenomenon. Regions come in all sizes but there is a tendency of correlated lattices to percolate more than similar uncorrelated lattices.

Percolation in terms of h_g does not discriminate well between percolation in correlated diluted triangular lattices and percolation in uncorrelated diluted triangular lattices. This is disappointing since for square lattices there was a clear difference in terms of h_g. However, parameter t_g is better suited to discriminate the percolation properties of these two lattices. This means that percolation in diluted lattices obtained after removing all frustration is better described in terms of the fractional bond content of the largest unfrustrated region t_g.

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