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Thermal operators in Ising percolation

M Caselle and F Gliozzi

Dipartimento di Fisica Teorica dell'Università di Torino, Istituto Nazionale di Fisica Nucleare, Sezione di Torino via P Giuria 1, I-10125 Torino, Italy

E-mail: caselle@to.infn.it and gliozzi@to.infn.it

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Abstract. We discuss a new cluster representation for the internal energy and the specific heat of the d-dimensional Ising model, obtained by studying the percolation mapping of an Ising model with an arbitrary set of antiferromagnetic links. Such a representation relates the thermal operators to the topological properties of the Fortuin–Kasteleyn (FK) clusters of Ising percolation and is a powerful tool to get new exact relations on the topological structure of FK clusters of the Ising model defined on an arbitrary graph.

1. Introduction

It is well known that the Ising model can be mapped into a percolation problem [1, 2]. In its original formulation this mapping is based on the identification of the mean value of the magnetization of the Ising model with the size of a (suitably defined) percolating cluster. Such identification is highly non-trivial and allows for a geometric characterization of several statistical observables near the critical point, a fact which has greatly improved our understanding of the Ising model and inspired new powerful algorithms [3, 4] to simulate the model. This mapping can also be extended to the thermal sector of the model, and cluster representations of, for instance, the internal energy and the specific heat can be easily constructed. However, in contrast to the case of magnetization, these representations are rather trivial and do not add any new geometrical or topological information to the model.

In this paper we shall discuss a new cluster representation for the thermal sector of the Ising model. To this end we shall first need to extend the percolation mapping to the case of the Ising model frustrated by some antiferromagnetic links [5] and then we use this mapping to extract a useful piece of information on the structure of the Fortuin–Kasteleyn (FK) clusters of the unfrustrated model.

The main feature of our new representation is that it relates the thermal operators of the model (in particular, the internal energy and the specific heat) to the topological properties of the clusters of a typical configuration of Ising percolation. As a consequence, one can write exact relations on the topological structure of the FK cluster.

The simplest of these new relations deals with the concept of non-cutting or *black* bond. A bond of a FK cluster is said to be black if its cancellation does not split the cluster in two disjoint parts. We shall prove (see section 6) that in the Ising model defined on an arbitrary

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d-dimensional lattice with N links at the coupling β, the mean number $\langle N_B \rangle$ of black bonds is related to the internal energy E by

$$E = \langle N_B \rangle \frac{1}{\sinh 2\beta} + N \tanh \beta. \tag{1}$$

Combining this with the well known expression (see equation (9))

$$E = \langle N_G \rangle \frac{e^{\beta}}{\sinh \beta} - N \tag{2}$$

where $\langle N_G \rangle$ is the mean number of bonds of FK graphs associated to the configurations of Ising percolation, yields a simple, exact relation between $\langle N_B \rangle$ and $\langle N_G \rangle$. Similar relations can be found for the specific heat.

In fact, these new relations are true for the Ising model defined on any arbitrary graph; however, in extracting our results we shall always assume for simplicity that the model is defined on a regular lattice in $d = 2, 3, \ldots$ dimensions with periodic boundary conditions boundary conditions (BCs).

In the process of constructing our new representation we shall discuss two issues which are rather interesting in themselves.

First, we shall construct a scheme to classify the bonds of a cluster on the basis of their topological properties (see section 3). The standard classification [6], which splits the bonds in three classes (which are commonly denoted with the three colours red, blue and green), refers to the bonds of the (infinite) percolating cluster. Our new representation of thermal operators suggests a slightly different bond partition, based on the connection properties of *all* the clusters. Within our classification scheme the topological properties of the bonds are unambiguously identified by the class to which they belong.

Second, we shall show in section 4.1, using duality, that in the Ising model all the correlators of an even number of spins (and hence invariant under the Z_2 symmetry of the model) can be expressed as ratios of partition functions with a suitable set of antiferromagnetic links.

This paper is organized as follows. The first part of the paper is composed of an introductory section on the Ising model and the percolation map (section 2) which will allow us to fix notation and to make the paper as self-contained as possible. In section 3 we discuss the topological properties of the clusters. In section 4 we deal with the Ising model in the presence of antiferromagnetic links and duality transformation, and section 5 is devoted to the extension of the percolation mapping to the frustrated Ising model. In these last two sections we have collected most of our new results which are then used in section 6 to construct new cluster representations for the internal energy and specific heat. Finally, section 7 is devoted to some concluding remarks.

2. Ising model

The d-dimensional Ising model is defined by the Hamiltonian

$$H(J, h') = -J \sum_{\langle n,m \rangle} s_n s_m + h' \sum_n s_n \tag{3}$$

where the field variable s_n takes the values -1 and $+1$; n labels the sites of the lattice (denoted by Λ in the following) which we assume to be a d-dimensional simple (hyper)cubic lattice of size L with periodic boundary conditions; however, a large part of our considerations are valid for an Ising model defined on an arbitrary graph. The notation $\langle n, m \rangle$ indicates that the sum is taken on nearest neighbour sites only. The partition function is defined as usual by

$$Z = \sum_{s_n = \pm 1} e^{-\beta H(J,h')} \tag{4}$$

where $\beta \equiv \frac{1}{kT}$. Plugging equation (3) in the definition of Z and assuming the usual conventions, $J = 1$ and $h = \beta h'$, we obtain

$$Z(\beta, h) = \sum_{s_n = \pm 1} \mathrm{e}^{\beta \sum_{\langle n,m \rangle} s_n s_m + h \sum_n s_n}. \tag{5}$$

For $h = 0$ and $d \geqslant 2$ the phase diagram of the model is composed of two phases separated by a second-order phase transition located at $\beta_c \equiv \frac{1}{kT_c}$. In the high-temperature phase the Z_2 symmetry of the model is preserved and the magnetization is zero; in the low-temperature phase the Z_2 symmetry is spontaneously broken and the magnetization becomes different from zero.

2.1. Mapping to a percolation model

In this section we shall discuss the mapping in the case $h = 0$. The extension to a nonzero magnetic field is straightforward and can be found, for instance, in [7].

The Ising partition function of equation (5) with $h = 0$ can be rewritten as

$$Z(\beta) = \mathrm{e}^{N\beta} \sum_{s_i = \pm 1} \prod_{\langle ij \rangle} [\mathrm{e}^{-2\beta} + (1 - \mathrm{e}^{-2\beta}) \delta(s_i, s_j)] \tag{6}$$

where $N \equiv dL^d$ is the number of links in the lattice and the δ function takes the value $\delta(s_i, s_j) = 1$ when the two arguments coincide and zero otherwise. Expanding the products in equation (6) one finds

$$Z(\beta) = \mathrm{e}^{N\beta} \sum_G \sum_{s_i = \pm 1} \left[\prod_{\langle ij \rangle \in G} p \delta(s_i, s_j) \right] (1 - p)^{N - N(G)} \tag{7}$$

where $p = 1 - \mathrm{e}^{-2\beta}$, G denotes an arbitrary subgraph of the lattice and $N(G)$ is the number of links of G. In general, G will be composed of several connected components (FK clusters in the following). Let us call $C(G)$ the number of clusters in the graph G. Note that among the clusters one has to also consider those with one site only.

Summing on the spin configurations in equation (7) we end up with

$$Z(\beta) = \mathrm{e}^{N\beta} \sum_G p^{N(G)} (1 - p)^{N - N(G)} 2^{C(G)} \tag{8}$$

which can be interpreted as the partition function of a percolation model with bond probability p and with a weight 2 for each independent cluster. In this framework the magnetization transition of the Ising model becomes a percolation transition, located at the percolation threshold $p_c \equiv 1 - \mathrm{e}^{-2\beta_c}$.

For $p > p_c$ an infinite, percolating cluster exists. The density of sites belonging to this percolating cluster, which is zero below p_c, can be used as order parameter for the percolation transition. It can be shown that it exactly coincides with the magnetization density of the original Ising model.

The internal energy in the percolation framework can be constructed by taking the logarithmic derivative of equation (8) with respect to β. The result is

$$E = \frac{2\langle N(G) \rangle}{p} - N \tag{9}$$

where the mean value is taken with respect to the measure of equation (8). It is interesting to compare this result with the standard definition of internal energy:

$$E = \frac{\partial}{\partial \beta} \log Z(\beta, h = 0) = \left\langle \sum_{\langle n,m \rangle} s_n s_m \right\rangle. \tag{10}$$

If we denote the number of links which join spins with the same sign in a given configuration by N_+ and the number of those which join spins with opposite sign by $N_- \equiv N - N_+$ then equation (10) can be rewritten as

$$E = \langle N_+ \rangle - \langle N_- \rangle = 2\langle N_+ \rangle - N. \tag{11}$$

By comparing equations (9) and (11) we see that

$$p\langle N_+ \rangle = \langle N(G) \rangle \tag{12}$$

which is the most intuitive way to define Ising percolation (and inspired Swendsen and Wang in their proposal [3]): given a generic configuration of the Ising model, delete all the bonds which join spins with opposite sign and, on the remaining graph, construct a standard percolation process, i.e. switch on the bonds at random with probability p. The resulting graph G will be a typical configuration of an Ising percolation model.

3. Cluster structure

As we have seen, an interesting feature of the percolation mapping is that it allows a geometric characterization of various thermodynamic quantities. In order to better understand this geometric setting it is convenient to study in a more precise and detailed way the cluster structure in a typical percolation configuration.

An important step in this direction was made by Stanley in 1977 [8] who noted that, at $p = p_c$, in a generic percolating cluster we can distinguish three different sets of bonds. By associating an electric unit resistance to each bond, and applying a voltage between the ends of the cluster, one can select the 'dangling bonds' (also called *green* bonds) which are those which do not carry current. The remaining bonds form the *backbone*; in this set one can then select the singly connected bonds (*red* bonds), which carry the whole current and have the property that if one is cut then the cluster breaks into two parts. The remaining bonds are multiply connected and are usually denoted as *blue* bonds. Starting from this coarse-grained classification, one can then look at more subtle structures, selecting, for instance, pairs of double connected bonds, triples .... Equivalently, one can look to the subsets of bonds which carry exactly half of the whole current, one-third, and so on.

With respect to this standard classification, which assumes free BCs, in this paper we prefer to deal with periodic BCs. This is because, as we shall see, the new representation of the thermal operators does not depend explicitly on the percolating property of the configurations, but rather on their winding and connection properties. We are then forced to introduce a different partition of the bonds which slightly differs from that of Stanley and applies not only to the (infinite) cluster wrapped along one or more directions, but also to any FK cluster contributing to the partition function.

We suggest that the reader follow our definitions looking at figure 1, where the bonds of a percolating cluster are split into three sets according to the Stanley classification (figure 1(*a*)) and ours (figure 1(*b*)).

G denotes the generic graph which appears in the sum of equation (8). It is composed of disconnected FK clusters. We call G_1 the set of those bonds which, when deleted, disconnect the cluster to which they belong into two disjoint clusters. Recall that we also consider as a cluster that composed of only one site and no bonds. We call the bonds of G_1 *grey* or *cutting* bonds.

Let us call G_0 the complement of G_1 in G, i.e. $G = G_0 \cup G_1$. G_0 contains two kinds of bonds: those which, if deleted, do not change the wrapping properties of G are called *black* bonds; those which transform a wrapped graph into an unwrapped one are called *red* bonds.

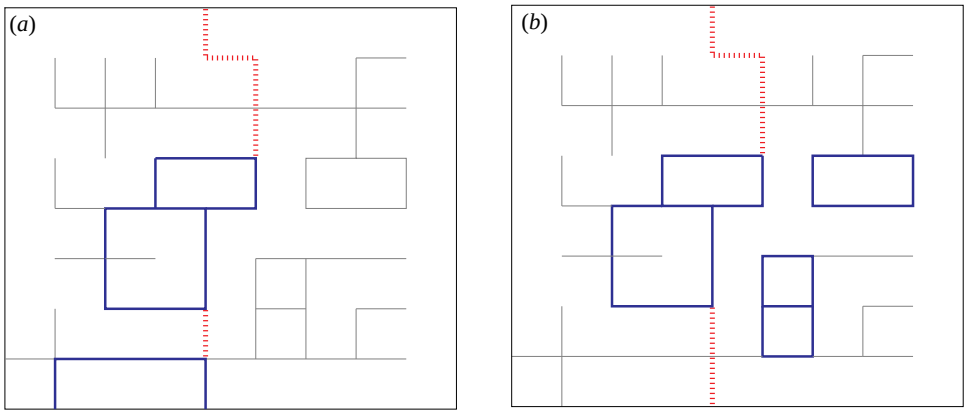

Figure 1. (*a*) Stanley classification of the bonds of a percolating cluster. The thin lines denote the dangling bonds, the thick lines the backbone and the dashed lines the red bonds. Free BCs are understood. (*b*) The same graph of figure 1(*a*) in the topological classification described in the text. Thin lines are the grey bonds, thick lines the black bonds and the dashed lines the red bonds. Periodic BCs are understood.

It is clear that our grey bonds form a subset of the dangling bonds of Stanley classification, but there are dangling bonds that are black in our classification, as comparison of figures 1(*a*) and (*b*) shows.

Using an electric circuit analogy again, one can say that our black and red bonds are those which carry current in the presence of a variable magnetic field pointing in a generic direction†.

It is known that the winding properties of the FK clusters are related to the interface tension in the low-temperature phase [10]. In this paper we shall see that the black bonds are directly involved in a new representation of the internal energy.

Our classification can be easily iterated by identifying other topological subsets of G_0 associated to other thermal observables. In particular, we need to define another set, denoted by H_2, that will play a major role in discussing the new representation of the specific heat. H_2 is the set of 'cutting pairs' of G_0, i.e. the set of those pairs of black bonds which, if simultaneously deleted, disconnect the cluster to which they belong into two separate clusters‡.

Let us examine a specific construction of the set H_2, which is interesting both because it sheds light on the structure of H_2 and because it can be straightforwardly iterated to construct 'cutting triplets' and from them possibly further higher combinations which contribute to higher derivatives of the free energy (in this paper, however, we shall not study these more complicated cases):

- Choose a link $l \in G_0$ and construct the graph $G_0(l)$ obtained from G_0 by deleting the link l.
- Select in $G_0(l)$ the cutting bonds (as we did above when we constructed G_1 starting from G), which form a set $G_1(l)$.
- Repeat the operation for all $l \in G_0$. The set of pairs $\{(l, h), \forall h \in G_1(l), \forall l \in G_0\}$ is exactly twice H_2 (due to the fact that each pair appears two times). This means that (apart

† We thank Lev Shchur for this observation.

‡ Note that, since by definition G_0 does not contain cutting bonds, at least two bonds are needed to disconnect a cluster.

from a factor two) H_2 coincides with the collection of graphs $G_1(l)$.

4. Ising model with a set of antiferromagnetic links

A natural extension of the Ising model discussed in section 2 is the one in which we allow the coupling J to change sign from link to link. Those links for which $J = -1$ are said to be antiferromagnetic or flipped links. In analogy with the definitions of section 2 (and setting for simplicity $h = 0$) we have now

$$H(J) = -\sum_{\langle n,m\rangle} J_{\langle n,m\rangle} s_n s_m \tag{13}$$

from which we may construct the partition function:

$$Z(\beta, J) = \sum_{s_n=\pm 1} \mathrm{e}^{-\beta\ S(J)}. \tag{14}$$

We denote the partition function without antiferromagnetic links and with periodic BCs by $Z(\beta)$. Denoting by F the set of flipped links we can write

$$\frac{Z(\beta, J_F)}{Z(\beta)} = \left\langle \prod_{\langle ij\rangle \in F} \mathrm{e}^{-2\beta s_i s_j} \right\rangle \tag{15}$$

where the mean value is taken with respect to the standard, unfrustrated Ising Hamiltonian. It is almost evident that suitable linear combinations of these expectation values reproduce the whole even sector of the theory. This can be simply proved using the Kramers–Wannier duality; this transformation gives a one-to-one map between these expectation values and the set of all correlation functions among the physical observables of the even sector of dual theory, as described in the next section.

4.1. Duality and frustrations

The Ising model defined in section 2 is characterized by the two following features: the dynamical variables (the spins) live on the *sites* and the interaction is defined on the *links* of the lattice Λ. Sites and links are respectively zero- and one-dimensional simplexes of the lattice. We can easily generalize the Ising model by looking to different geometrical realizations of dynamical variables and interaction Hamiltonians. For instance, in the Ising gauge model we take the spins $\tilde{s}_l$ to live on links l and the interaction to be defined on plaquettes $\tilde{s}_{\square} = \prod_{l\in\square} \tilde{s}_l$. We could also choose the dynamical variables on the plaquettes and the Hamiltonian to live on cubes, thus defining a Kalb–Ramond-type theory.

It is well known that the Kramers–Wannier duality transformation can be generalized to Ising models in any dimension d. This transformation is not a symmetry of the model: it maps one description of the dynamical system to another description of the *same system*. This duality transforms a given lattice Λ (in our case the (hyper)cubic lattice on which the Ising model is defined) into a new lattice (the dual lattice $\tilde{\Lambda}$) in which each k-dimensional simplex is mapped to a $d-k$ one. In the case of (hyper)cubic lattices the dual lattice again turns out to be (hyper)cubic.

Under this mapping the Ising model on Λ is transformed into a new model whose Hamiltonian lives on a $d-1$ simplex of $\tilde{\Lambda}$. Thus we have the following correspondences:

if $d = 2$ Ising model $\Longleftrightarrow$ Ising model

if $d = 3$ Ising model $\Longleftrightarrow$ Z_2 gauge model

if $d = 4$ Ising model $\Longleftrightarrow$ Z_2 Kalb–Ramond model.

It can be shown that in the thermodynamic limit the free energy density of the original Ising model coincides (apart from an additive function of β which can be evaluated exactly) with that of the dual model evaluated at the dual coupling $\tilde{\beta}$ defined as

$$\tilde{\beta} = -\tfrac{1}{2}\log[th(\beta)]. \tag{16}$$

Using a duality transformation it is possible to build up a one-to-one mapping between a given pattern $J = \{J_{\langle ij\rangle}\}$ of antiferromagnetic links and the correlators of the physical observables of the dual description. Take, for instance, the three-dimensional case and denote by F the set of flipped links. Associate to each of these links the corresponding plaquette of the dual lattice and denote by $\tilde{F}$ this set. Duality implies that†

$$\left\langle \prod_{\langle ij\rangle\in F} \mathrm{e}^{-2\beta s_i s_j} \right\rangle = \left\langle \prod_{\tilde{\square}\in\tilde{F}} \tilde{s}_{\tilde{\square}} \right\rangle_{\text{gauge}} \tag{17}$$

where the left-hand side coincides with the ratio of the partition functions defined in equation (15), while the right-hand side is the expectation value of the product of plaquette variables $\tilde{s}_{\tilde{\square}}$ with a Boltzmann factor $\mathrm{e}^{-\tilde{\beta}S_{\text{gauge}}}$ with

$$S_{\text{gauge}} = -\sum_{\tilde{\square}} \tilde{s}_{\tilde{\square}} \qquad \tilde{s}_{\tilde{\square}} = \tilde{s}_{l_1}\tilde{s}_{l_2}\tilde{s}_{l_3}\tilde{s}_{l_4} \tag{18}$$

where $\tilde{s}_l \in \{1, -1\}$ are the variables located in the links of $\tilde{\Lambda}$.

Conversely, given any product of Wilson loops $W(C1)W(C2)\ldots$, we can replace it (in many ways) with an equivalent set of elementary plaquettes, with the only constraint that the boundary of this set should coincide with the set of loops $\{C1, C2, \ldots\}$; then we can again apply equation (17) and this completes the proof of the above-mentioned one-to-one correspondence in the three-dimensional case. The extension to other dimensions is straightforward.

We now want to use this correspondence to show that for the even sector of the spin Ising model (namely for the operators obtained as products of an even number of spins and hence invariant under the Z_2 symmetry of the model) the set of ratios (15) corresponding to all the possible choices of antiferromagnetic bonds forms a complete set in the sense that any correlator of the spin Ising model can be expressed in terms of these ratios. To be definite we put forward this argument for the three-dimensional case again, its generalization to other dimensions being straightforward. The set of products of Wilson loops forms a complete set of observables of the dual description; the simplest, non-trivial observable is the plaquette. The spin–spin correlators on the original lattice Λ can be expressed in terms of the gauge model by flipping the set of plaquettes of $\tilde{\Lambda}$ intersected by a path $\gamma \subset \Lambda$ connecting the site x to the site y:

$$\langle s_x s_y\rangle = \left\langle \prod_{\tilde{\square}\in\gamma} \mathrm{e}^{-2\tilde{\beta}\tilde{s}_{\tilde{\square}}} \right\rangle_{\text{gauge}}. \tag{19}$$

Using the obvious identity $\mathrm{e}^{-2\tilde{\beta}\tilde{s}_{\tilde{\square}}} = \cosh 2\tilde{\beta} - \sinh 2\tilde{\beta}\tilde{s}_{\tilde{\square}}$, the right-hand side can be written as a combination of expectation values of products of Wilson loops. Then using equation (17) we can evaluate this correlator directly in the Ising model in terms of flipped partition functions. Such a construction can be repeated for any other spin correlator and easily generalized to any dimension d. In conclusion, we can state that the whole set of spin correlators of the Ising model in any dimension can be encoded in a suitable set of ratios of flipped partition functions.

† It is important to stress that equation (17) holds only in the thermodynamic limit, in which the BCs can be neglected. In fact, in general the duality transformation does not preserve specific choices of the BCs. In particular, periodic BCs are mapped by duality into a mixture of periodic and antiperiodic BCs.

5. Percolation mapping of the frustrated model

The percolation mapping discussed in section 2.1 can also be extended to the frustrated Ising model [5]†. The main difference with respect to the unfrustrated case is that now the topology of the cluster is also important. Let us examine this mapping in detail.

We assume that the set of couplings J_{ij} of equation (3) is given by an arbitrary, fixed collection of signs ± 1. As in the case without frustrations the Ising partition function of equation (14) can be rewritten as

$$Z(\beta, J) = \mathrm{e}^{N\beta} \sum_{s_i=\pm 1} \prod_{\langle ij \rangle} [1 - p + p\delta(J_{\langle ij \rangle} s_i s_j)] \tag{20}$$

where $\delta(J_{\langle ij \rangle} s_i s_j) \equiv (1 + J_{\langle ij \rangle} s_i s_j)/2$ is a projector on configurations with $J_{\langle ij \rangle} s_i s_j = 1$. Expanding the products in equation (20) we find that

$$Z(\beta, J) = \mathrm{e}^{N\beta} \sum_{G} (1-p)^{N-N(G)} p^{N(G)} \sum_{s_i=\pm 1} \left[\prod_{\langle ij \rangle \in G} \delta(J_{\langle ij \rangle} s_i s_j) \right]. \tag{21}$$

As in section 2, N is the total number of links of the lattice, the summation goes over all the subgraphs G of the lattice, $N(G)$ is the number of links of G and $p = 1 - \mathrm{e}^{-2\beta}$.

Note that the whole dependence on the signs $J_{\langle ij \rangle}$ is contained in the δ projectors and that the product inside the square brackets is a projector which forces all the links of each connected component G_c of the graph to fulfil the constraint

$$J_{\langle ij \rangle} s_i s_j = 1 \qquad \langle ij \rangle \in G_c. \tag{22}$$

We say that a cluster G_c is *compatible* with a given choice of couplings $J_{\langle ij \rangle}$ if there is a configuration of its sites obeying such a constraint. In the standard case ($J_{\langle ij \rangle} = 1 \; \forall \langle ij \rangle$) this condition implies simply that the sites of each cluster have the same sign. In the presence of frustrations it is easy to verify that equation (22) is a topological constraint, telling us that a connected graph G_c is compatible if and only if no loop of G_c includes an odd number of antiferromagnetic links.

A crucial observation is that, owing to the connected nature of the cluster, the value of s_i of any site i of a compatible cluster fixes the values of all the other sites of the cluster, and that if $\{s_i, i \in G_c\}$ is a solution of the constraint, the opposite configuration $\{-s_i\}$ is also a solution. Thus any connected subgraph contributes to the partition function with a factor of two if it is a compatible cluster, otherwise it gives a zero contribution. Thus summing on the spin configurations in equation (21) we end up with

$$Z(\beta, J) = \mathrm{e}^{N\beta} \sum_{G} \varpi_J(G) p^{N(G)} (1-p)^{N-N(G)} 2^{C(G)} \tag{23}$$

where ϖ_J denotes the projector on compatible graphs, i.e. graphs made with compatible clusters, defined as follows:

$$\varpi_J(G) = \begin{cases} 1 & \text{if no loop of } G \text{ contains an odd} \\ & \text{number of antiferromagnetic links,} \\ 0 & \text{otherwise.} \end{cases} \tag{24}$$

In the standard, unfrustrated case the sum over G is unconstrained and we obtain the result discussed in section 2.1. When there are frustrations, the set of compatible graphs is a proper

† See also [9] for some recent application of the percolation mapping in the presence of frustrations to the study of disordered systems.

subset of the all the possible subgraphs of the lattice. We can then write the following exact relation, which is the cluster version of the equation (15):

$$\frac{Z(\beta, J)}{Z(\beta)} = \langle \varpi_J \rangle \tag{25}$$

where the expectation value is taken with respect to the standard Hamiltonian.

An interesting, particular example is the Ising model on a cubic lattice with periodic (p) BCs in one coordinate direction, say z, in which all the links of a slice orthogonal to z are flipped to -1. Such a pattern of antiferromagnetic couplings is equivalent to choosing antiperiodic BCs (a) along the z direction. Denoting with Z_a and Z_p the partition functions with these two different choices of boundary conditions, we have

$$\frac{Z_a}{Z_p} = \langle \varpi_z \rangle \tag{26}$$

where ϖ_z is a projector on the FK graphs which is 1 if there is no cluster with an odd winding number in the z direction and 0 otherwise. Equation (26) is the starting point of a new representation of the interface free energy first found in [10] which is particularly useful near the critical point.

Coming back to the general formula (25), we would like to make a few comments:

- Equation (25) is valid not only for any regular lattice in any dimension, but also for the Ising model defined on an arbitrary graph and for any choice of antiferromagnetic couplings.
- Any correlator of the even sector of the Ising model can be expressed in terms of the ratios (25).
- The projector ϖ_J depends only on the subgraph $G_0 \subset G$.

As a consequence, there is no information loss in the even sector if one deletes all the grey bonds of any graph G, provided one uses equation (25) to evaluate these observables. In other words, in the partition function (8) we can split the sum over all possible graphs $\sum_G$ as the double sum

$$Z(\beta) = \mathrm{e}^{N\beta} \sum_{G_0} \sum_{G_1(G_0)} p^{N(G)} (1-p)^{N-N(G)} 2^{C(G)} \equiv \sum_{G_0} \mathrm{e}^{-\mathcal{H}(G_0;\beta)} \tag{27}$$

where $G = G_0 \cup G_1$ and $G_1(G_0)$ denotes an arbitrary set of grey bonds compatible with a fixed set G_0 of black (and red) bonds. $\mathcal{H}$ defines a new Hamiltonian which depends only on the configurations of the black bonds. Equation (25) tell us that, in spite of the sum over all the possible insertions of grey bonds, exactly the same piece of information about the even sector is encoded in the resulting Hamiltonian $\mathcal{H}$ as in the original Ising Hamiltonian. Although this fact will not be exploited in this paper, it clearly suggests the existence of a huge hidden symmetry of the theory.

6. Cluster description of thermal observables

We are now in a position to study a new cluster representation of thermal observables, alternative to the one presented at the end of section 2.1. Let us look first at the internal energy.

6.1. Internal energy

Let us consider an Ising system defined on an arbitrary lattice in d space dimensions with only one antiferromagnetic link in the position $\langle ij \rangle$. Then equation (15) can be rewritten explicitly as

$$\frac{Z(\beta, J_{\langle ij \rangle})}{Z(\beta)} = \langle \mathrm{e}^{-2\beta s_i s_j} \rangle = \cosh 2\beta - \langle s_i s_j \rangle \sinh 2\beta. \tag{28}$$

On the other hand, using equation (25) we get

$$\langle s_i s_j \rangle = \text{cotanh}2\beta - \frac{\langle \varpi_{\langle ij \rangle} \rangle}{\sinh 2\beta} \tag{29}$$

where $\varpi_{\langle ij \rangle}$ is the projector on the graphs compatible with the antiferromagnetic link in the position $\langle ij \rangle$. Such graphs are of two types:

- those in which the link $\langle ij \rangle$ does not appear;
- those in which the cluster which contains the bond $\langle ij \rangle$ is split into two separate clusters when it is deleted.

These two conditions tell us simply that $\langle ij \rangle$ does not belong to the subgraph G_0 of G. Summing over all the possible links and taking advantage of the translational invariance of the lattice we find that

$$\left\langle \sum_{\langle n,m \rangle} \varpi_{\langle nm \rangle} \right\rangle = N - \langle N(G_0) \rangle. \tag{30}$$

Combining this result with equations (29) and (10) we get the sought-after representation of the energy in terms of black bonds:

$$E = \frac{\langle N(G_0) \rangle}{\sinh(2\beta)} + N \tanh \beta, \tag{31}$$

as anticipated in the introduction. This is the first main outcome of our analysis.

6.2. Specific heat

Let us start from the following definition of the specific heat:

$$C = \left\langle \left(\sum_{\langle n,m \rangle} s_n s_m \right) \left(\sum_{\langle k,l \rangle} s_k s_l \right) \right\rangle - \left\langle \left(\sum_{\langle n,m \rangle} s_n s_m \right) \right\rangle^2. \tag{32}$$

Call $f = \langle nm \rangle$ and $g = \langle kl \rangle$ the two links and separate the case $f = g$ in the sum. We obtain

$$C = \left(N - \frac{E^2}{N} \right) + \sum_{f \neq g} [\langle s_f s_g \rangle - \langle s_f \rangle \langle s_g \rangle] \tag{33}$$

with $s_f \equiv s_m s_n$ and $s_g \equiv s_k s_l$.

In order to get the new cluster representation of C it is sufficient to now consider a system with two antiferromagnetic links located in f and g with the associated projector ϖ_{fg}. Then we have

$$\langle \varpi_{fg} \rangle \equiv \langle \mathrm{e}^{-2\beta(s_f + s_g)} \rangle = \langle (\cosh 2\beta - s_f \sinh 2\beta)(\cosh 2\beta - s_g \sinh 2\beta) \rangle. \tag{34}$$

Again using equation (29) we get

$$\sum_{f \neq g} [\langle s_f s_g \rangle - \langle s_f \rangle \langle s_g \rangle] = \sum_{f \neq g} \frac{\langle \varpi_{fg} \rangle - \langle \varpi_f \rangle \langle \varpi_g \rangle}{\sinh^2 2\beta}. \tag{35}$$

The graphs with $\varpi_{fg} = 1$ are of two types:

- Those in which both f and g do not belong to the G_0 subgraph; when summing over f and g these configurations give simply the contribution $\sum_{fg} \varpi_f \varpi_g = (N - N(G_0))(N - N(G_0) - 1)$.
- Those in which both f and g belong to G_0 but are such that any loop going through f contains also g. Let us denote by $\mathcal{G}_{fg}$ the projector which selects the graphs with this special property.

We may give a cluster representation of the specific heat if we are able to evaluate the sum $\sum_{f\neq g}\mathcal{G}_{fg}$. Reversing the order of summations, i.e. taking first the sum over all the pair of links and then the sum over G implied in the expectation value we obtain

$$\sum_{f\neq g}\langle\mathcal{G}_{fg}\rangle = 2\langle N(H_2)\rangle. \tag{36}$$

In fact, from the definition of $\mathcal{G}_{fg}$, if $\mathcal{G}_{fg}=1$ then cutting simultaneously f and g we disconnect the cluster to which they belong into two subclusters, and conversely if two links belong to G_0 and are a cutting pair then they certainly fulfil the condition $\mathcal{G}_{fg}=1$. The factor two is due to the fact that in the sum the pair f, g appears twice.

Collecting together the various pieces we end up with

$$C = \left(N - \frac{E^2}{N}\right) + \frac{2\langle N(H_2)\rangle + \sum_{f\neq g}(\langle\varpi_f\varpi_g\rangle - \langle\varpi_f\rangle\langle\varpi_g\rangle)}{\sinh^2(2\beta)} \tag{37}$$

which gives the new representation of the specific heat in terms of black bonds.

7. Conclusions

In this paper we have shown how to construct a new representation of thermal operators in Ising percolation in terms of a new set of bonds, called the black bonds, forming a subset of the standard FK clusters. Our approach is quite general; indeed, we never needed to specify the lattice structure. In fact, our results are also true for Ising models defined on arbitrary graphs.

Our main results are:

- We proposed a new scheme to classify the bonds of a cluster on the basis of their topological properties. We have discussed the relations with the standard classification scheme.
- We pointed out that in the Ising model all the correlators of an even number of spins can be expressed as ratios of partition functions with flipped links. In particular, we have applied this result to the internal energy and the specific heat.
- We found that in the configurations of black bonds contributing to the partition function is encoded the whole information on the even sector of the theory; in particular, that the internal energy can be expressed in terms of the mean number of black bonds and that the specific heat is related to their variance and to the special subset H_2 defined in section 3.
- Finally, we observed that our new representation of observables of the even sector suggests the existence of a huge hidden symmetry of the Ising model.

Our results can be straightforwardly extended to q-state Potts models with generic values of q [14].

The most relevant application of the present analysis is that it may help to find new powerful algorithms to simulate the Ising model or to construct improved estimators for thermal observables. As a matter of fact, for some special configurations of antiferromagnetic links these algorithms already exist. In the case of a whole flipped hyperplane leading to antiperiodic BCs this possibility was discussed for the first time by Hasenbusch in [10], who provided a very powerful tool to evaluate the surface tension. Later, it was modified so as to evaluate in the dual version Wilson loops [11], correlators of Polyakov loops [12] and plaquette expectation values [13] in the gauge Ising model. We hope that the present analysis might help to further extend the range of these applications.

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