

The Discrete N -Vector Ferromagnet: Connection to a Percolation with Frustration Features

by

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ABSTRACT

We extend the Kasteleyn-Fortuin formalism to the discrete N -vector ferromagnet. We show that the free energy and the correlation functions of this model are related, when the number of states tends to 1, to the mean number of clusters and to the pair connectedness of a polychromatic bond percolation type problem, which combines frustration and connectivity features.

Key-words: Percolation; Discrete N -vector model.

1 Introduction

The establishment of connections between lattice statistical models and percolation type problems⁽¹⁻¹⁵⁾ has proved to be very fruitful. On the one hand, it has enhanced the understanding of critical phenomena in terms of geometrical concepts. On the other hand it allows the various techniques developed in the theory of thermal critical phenomena to be used in the study of percolation problems. Moreover, these geometric formulations of thermal statistical models provide the basis of construction of *cluster* dynamics which can drastically reduce the critical slowing down in Monte Carlo simulations of these models (see^{(16),(17)} and references therein). For example, in the case of the Potts ferromagnet⁽¹⁸⁾, Swendsen and Wang⁽¹⁶⁾ have introduced such a cluster dynamics based on the Kasteleyn and Fortuin (KF)⁽¹⁾ formalism. In this dynamics, all the spins belonging to the same cluster are flipped in a single step, contrarily to single spin dynamics where the spins are flipped one at a time. The above reduction of the relaxation time stems from the fact that all the spins of such clusters are *correlated* and can, thus, be treated as single spins, with no need of waiting for single spin fluctuations to propagate over large correlated regions.

The mentioned percolation formulations of spin models have been developed, for example, for the pure Potts model^{(1,2,5)(8-10)}, dilute Potts model^(6,7), Potts model with multisite interactions^(3,4), chiral Potts model types⁽¹¹⁾, q-state frustrated Potts model^(12,13), mixed flow models and mixed potential-difference models⁽¹⁴⁾, XY (or more generally $O(n)$) models⁽¹⁵⁾. Many of these formulations involve two main steps. Firstly, the partition function and correlation functions of the considered spin model are written in terms of percolation average types of quantities which depend on the number λ of spin states. Secondly, geometric properties of the corresponding percolation problem (such as the mean number of clusters, pair connectedness, etc.) are derived from the above percolation averages in the $\lambda \rightarrow 1$ limit (or, $\lambda \rightarrow 0$ when loops are not allowed). In some complex cases, one does not succeed in accomplish the second step. In our knowledge, the global two-step geometrical formulation for the discrete N-vector model has not, in our knowledge, been reported in the literature. This model, also called the discrete N-component cubic model, was firstly introduced by Kim et al⁽¹⁹⁾ in order to account for the unusually large specific heat critical exponents which have been observed in phase transitions in cubic rare earth compounds, like in HoSb. It has many other realizations such as the order-disorder transition in atomic oxygen on tungsten⁽²⁰⁾, the orientational ordering of diatomic molecules adsorbed on a triangular lattice⁽²¹⁾ (as observed in N_2 adsorbed on graphite⁽²²⁾), etc. This model was, afterwards, extended⁽²³⁾ in order to include quadrupolar interactions, besides

the dipolar ones. This generalized model, which we will simply refer to, henceforth, as the *cubic model* is a discrete version of the continuous N -component cubic model. Under the theoretical point of view, it has been studied through many different methods (see, for example,⁽²⁴⁾ and references therein) and it contains several important statistical models, namely, the Ising model ($N = 1$), the $Z(4)$ model ($N = 2$), the self-avoiding walk ($N \rightarrow 0$)⁽²⁵⁾ and the Potts model. Furthermore, for a general value of N , the cubic model is a particular case of the $Z(\lambda)$ model ($\lambda = 2N$), which plays an important role in both lattice gauge theory and statistical mechanics (see, for example,⁽²⁶⁾ and references therein).

Herein, we develop a two-step geometrical formulation of the cubic model through a procedure similar to the one introduced by Kasteleyn and Fortuin⁽¹⁾ for the Potts model. We prove that, in the $\lambda = 2N \rightarrow 1$ limit, the free energy and the correlations functions of the cubic model are related to the mean number of clusters and pair connectedness of a new kind of polychromatic bond percolation⁽²⁷⁾. In this problem there are three types of present bonds, say green, yellow and blue ones, which can be conveniently pictured as being negative (green) and positive (yellow or blue) bonds. The new feature of this percolation is the fact that only the configurations which do not have any *frustration* are allowed.

This paper is divided as follows. In section 2, we define the model and summarize previous results for both the $Z(\lambda)$ and cubic models which will be used in the subsequent parts. In section 3, we express the partition function and the correlation functions of the cubic model as polychromatic bond percolation averages containing two types of present bonds. In section 4, we transform these averages in other ones in such a way that they lead, in the $\lambda = 2N \rightarrow$ limit, to a new kind of percolation problem. We also show that our results recover the KF ones in the appropriate limits corresponding to the Ising and Potts models. The conclusions are given in section 5. Finally, we give in the Appendix the proof of a fundamental relation necessary to transform the formulation of section 3 into that of section 4.

2 The Cubic and Related Models

2.1 The Discrete Cubic Model

Let us consider the discrete N -component cubic model on a graph G with vertex set V , edge set E , number of vertices $|V|$ and number of edges $|E|$. (We shall use throughout

this paper the notation $|A|$ to indicate the number of elements of a set A). We associate with each vertex i of V a N -component vector \vec{S}_i which can point into one of the $2N$ directions (positive and negative) of the Cartesian axes in a N -dimensional space, in other words:

$$\vec{S}_i = (\pm 1, 0, \dots, 0) \quad \text{or} \quad (0, \pm 1, 0, \dots, 0) \quad \text{or} \quad \dots (0, 0, \dots, 0, \pm 1) \quad (1)$$

Then, one can describe the discrete cubic model by the following dimensionless Hamiltonian⁽²³⁾:

$$\beta \mathcal{H}(G) = - \sum_{e \in E} \{ NK_e \vec{S}_i \cdot \vec{S}_j + NL_e (\vec{S}_i \cdot \vec{S}_j)^2 \} \quad (\beta \equiv 1/k_B T) \quad (2)$$

where K_e and L_e are the respective dimensionless coupling constants associated with the dipolar and quadrupolar interactions between spins \vec{S}_i and \vec{S}_j located at the vertices i and j of the edge e . The above sum is over all interacting pairs of spins on G .

Notice that for a spin \vec{S}_i which lies along the Cartesian axis x_ℓ ($\ell = 1, 2, \dots, N$), its α^{th} component $S_{i\alpha}$ ($\alpha = 1, 2, \dots, N$) is given by:

$$S_{i\alpha} = \sigma_i \delta(\ell, \alpha) \quad (\alpha = 1, 2, \dots, N; \sigma_i = \pm 1) \quad (3)$$

where $\sigma_i = \pm 1$ specifies the sense ($x_\ell \gtrless 0$) of the spin, and $\delta(\ell, \alpha)$ is the Kronecker function. In fact, one can regard (see⁽²³⁾) the discrete cubic model as that in which one associates to each vertex i of the graph G two coupled variables: an Ising one ($\sigma_i = \pm 1$) and a N -state Potts one ($\alpha_i = 1, 2, \dots, N$).

The discrete cubic model contains several particular cases. It becomes for $N = 1$ and 2 identical, respectively, to the Ising model and the symmetric Ashkin-Teller model⁽²⁸⁾ (or, equivalently, the $Z(4)$ model). It reduces, for $K_e = L_e$, to a $2N$ -state Potts model (with coupling constant $2NK_e$). Another special case occurs when $K_e = 0$, which corresponds to a N -state Potts model (with coupling constant NL_e) and $|V|$ independent $S = 1/2$ spins. Although these independent spins have been disregarded in the literature as they lead to just a zero-energy shift, they are important herein for checking if our results recover, as particular cases, the appropriate ones. The studied model contains also the self-avoiding walk with fugacity K_e in the $N \rightarrow 0$ limit⁽²⁵⁾. Finally, when $L_e/|K_e| \rightarrow \infty$ all spins are induced to be parallel or anti-parallel ($\vec{S}_i \cdot \vec{S}_j = \pm 1 \forall_{i,j}$) and the cubic model reduces to N decoupled Ising models, each one being along one of the Cartesian axes and having coupling constant NK_e .

2.2 Known Results for the $Z(\lambda)$ and Discrete Cubic Models

The $Z(\lambda = 2N)$ model, which is related to the N -component discrete cubic model, is defined by the following dimensionless Hamiltonian for a graph G (with vertex set V and edge set E):

$$\beta\mathcal{H}(G) = \sum_{e \in E} h_e(n_i - n_j) \quad (4)$$

where n_i is the state variable associated with each vertex i of V which can take on one of the $\lambda = 2N$ integer values $0, 1, \dots, \lambda - 1$. $(n_i - n_j)$ is calculated mod- λ and the pair interaction energy depends only on the relative ordering of i and j , i.e.

$$h_e(\lambda - \alpha) = h_e(\alpha) \quad (\forall \alpha = 0, 1, \dots, \lambda - 1) \quad (5)$$

An useful variable which has been used in many RG calculations is the *vector transmissivity* (see the review of⁽²⁹⁾ and references therein). In the case of the $Z(\lambda)$ model it is a λ -dimensional vector \vec{t}_e whose components $t_e(\alpha)$ are defined⁽³⁰⁾ by:

$$t_e(\alpha) = \frac{1}{z_e} \sum_{\beta=0}^{\lambda-1} e^{2\pi i \alpha \beta / \lambda} e^{-h_e(\beta)} \quad (\alpha = 0, 1, \dots, \lambda - 1) \quad (6.a)$$

where

$$z_e = \sum_{\alpha=0}^{\lambda-1} e^{-h_e(\alpha)} \quad (6.b)$$

Notice that only $Int(\lambda/2)$ (where Int stands for the integer part) components of $\vec{t}_e(\alpha)$ are independent since $t_e(0) = 1$ and $t_e(\lambda - \alpha) = t_e(\alpha)$.

If we associate a vector transmissivity \vec{t}_e with each edge e of the edge set E of G , we can define an *equivalent vector transmissivity* $\vec{T}(1, 2; G)$ between the roots¹ 1 and 2 of G as the vector transmissivity \vec{t}_{eff} of a single effective edge between 1 and 2 having an equivalent Hamiltonian $h_{eq}(n_1 - n_2)$ given by:

$$Tr' \left\{ \exp \left[- \sum_{e \in E} h_e(n_i - n_j) \right] \right\} = C \exp[-h_{eq}(n_1 - n_2)] \quad (7)$$

where C is a constant and Tr' denotes the trace over all possible configurations of n_i for all vertices i which are distinct from the roots 1 and 2.

It has been shown⁽³¹⁾ that this vector $\vec{T}(1, 2; G)$ is related to pair correlation functions. These functions can normally be written as the thermal average of some function $f(n_1 - n_2)$

¹Roots are vertices of a graph which play a special role; in the considered case they are the chosen vertices between which we calculate the equivalent vector transmissivity.

depending only on the difference, mod- λ , of the state variables n_1 and n_2 . It can be Fourier decomposed as⁽³¹⁾:

$$\overline{f(n_1 - n_2)} = \frac{1}{\lambda} \sum_{\alpha=0}^{\lambda-1} f_{\lambda-\alpha} T_{\alpha}(1, 2; G) \quad (8)$$

where the bar indicates a thermal average (such notation will be used henceforth). $T_{\alpha}(1, 2; G)$ is the α -component of the equivalent vector transmissivity $\vec{T}(1, 2; G)$ which is equal to:

$$T_{\alpha}(1, 2; G) = \overline{\exp[-2\pi i(n_1 - n_2)/\lambda]} = \frac{N_{\alpha}(1, 2; G)}{D(G)} \quad (9)$$

$N_{\alpha}(1, 2; G)$ and $D(G) = N_0(1, 2; G)$ are the respective numerator and denominator of $T_{\alpha}(1, 2; G)$ whose definitions in terms of mod- λ flows can be found in⁽³¹⁾.

$D(G)$, on the other hand, is related to the partition function $Z(G)$ through⁽³²⁾:

$$Z(G) = \lambda^{|V|-|E|} \left(\prod_{e \in E} z_e \right) D(G) \quad (10)$$

where z_e is defined in eq. (6b).

Let us now specialize the above results for the discrete N -component cubic model. The latter corresponds to the particular case of the $Z(2N)$ model in which $h_e(n_i)$ ($n_i = 0, 1, \dots, 2N - 1$) become highly degenerate⁽²⁴⁾, namely:

$$h_e(1) = h_e(2) = \dots = h_e(N - 1) = h_e(N + 1) = \dots = h_e(2N - 1) \quad (11)$$

and where the dimensionless coupling constants K_e and L_e are related to the energy differences through:

$$2NK_e = h_e(N) - h_e(0) \quad (12.a)$$

and

$$N(K_e + L_e) = h_e(1) - h_e(0) \quad (12.b)$$

The vector transmissivity (eq. 6) becomes in this case a two-component vector given by^(24,33):

$$t_e(\alpha) = \frac{1 - e^{-2NK_e}}{1 + 2(N - 1)e^{-N(K_e+L_e)} + e^{-2NK_e}} \equiv t_e(1) \quad (\alpha = 1, 3, \dots, 2N - 1) \quad (13.a)$$

and

$$t_e(\alpha) = \frac{1 - 2e^{-N(K_e+L_e)} + e^{-2NK_e}}{1 + 2(N - 1)e^{-N(K_e+L_e)} + e^{-2NK_e}} \equiv t_e(2) \quad (\alpha = 2, 4, \dots, 2N - 2) \quad (13.b)$$

Using eqs. (8) and (9) one can show⁽²⁹⁾ that the equivalent vector transmissivity $\vec{T}(1, 2; G) \equiv \{T_1(1, 2; G), T_2(1, 2; G)\}$ between the roots 1 and 2 of G is:

$$T_1(1, 2; G) = \frac{N_1(1, 2; G)}{D(G)} = \overline{\vec{S}_1 \vec{S}_2} \quad (14)$$

and

$$T_2(1, 2; G) = \frac{N_2(1, 2; G)}{D(G)} = \left(\frac{N(\vec{S}_1 \cdot \vec{S}_2)^2 - 1}{N - 1} \right) \quad (15)$$

One important property of $N_\alpha(1, 2; G)$ ($\alpha = 1, 2$) is the fact that it is zero whenever there is no path connecting the roots 1 and 2. $\vec{T}(1, 2; G)$ can be calculated through the traditional trace over configurations given by eq. (7) or, alternatively, through the break-collapse method^(24,33). This technique has the advantage of allowing the calculation of $\vec{T}(1, 2; G)$ (and hence of the above correlation functions) for cubic clusters for all values of N *simultaneously* without having to examine configurations. At the heart of this method is the effective break-collapse equation given by⁽²⁴⁾:

$$N_\alpha(1, 2; G) = N_1^{(j)} N_\alpha(1, 2; G_j^{cc}) + (D^{(j)} - N_2^{(j)}) N_\alpha(1, 2; G_j^{bb}) + \\ + (N_2^{(j)} - N_1^{(j)}) N_\alpha(1, 2; G_j^{(bc)}) \quad (\alpha = 0, 1, 2) \quad (16)$$

where G_j^{bb} , G_j^{cc} and G_j^{bc} are, respectively, the broken (where $t_1^{(j)} = t_2^{(j)} = 0$), the collapsed (where $t_1^{(j)} = t_2^{(j)} = 1$) and the precollapsed (where $t_1^{(j)} = 0$, $t_2^{(j)} = 1$) graphs and the edge j has a vector transmissivity $\vec{t}^j \equiv (t_1^{(j)} = N_1^{(j)}/D^{(j)}, t_2^{(j)} = N_2^{(j)}/D^{(j)})$. G_j^{bb} and G_j^{cc} are obtained from the graph G by deleting the chosen edge j and contracting it (i.e., identifying the endpoints of j in G_j^{bb}) respectively. In G_j^{bc} we do not change the topology of G ; we only alter the coupling constants associated with the edge j , setting them to $K_e = 0$ and $L_e \rightarrow \infty$. Notice that $N_0(1, 2; G) = D(G)$.

During the iterative application of this equation one may arrive at a graph G_{pr} whose edges are all precollapsed (we shall demoninate it a “precollapsed graph”). In this case, it has been proved⁽²⁴⁾ that such a graph is precollapsed itself with the following equivalent vector transmissivity:

$$N_1(1, 2; G_{pr}) = 0 \quad (17.a)$$

$$N_2(1, 2; G_{pr}) = N^{c(G_{pr})} \gamma_{12}(G_{pr}) \quad (17.b)$$

and

$$D(G_{pr}) = N^{c(G_{pr})} \quad (17.c)$$

where $c(G_{pr})$ is the cyclomatic number (i.e., number of independent cycles) of G_{pr} , and $\gamma_{12}(G_{pr})$ is 1 if the roots 1 and 2 are connected and zero otherwise. The cyclomatic number $c(G_{pr})$ can be calculated through the Euler relation valid for any graph G , namely:

$$c(G) = |E| - |V| + w(G) \quad (18)$$

where $w(G)$ is the number of clusters in G (including the isolated vertices).

3 Polychromatic Percolation Average Forms for the Partition and Correlation Functions

In this section we shall express the partition function and the correlation functions of the discrete cubic model as standard polychromatic bond percolation averages. For this, we shall follow along the lines of Kasteleyn and Fortuin⁽¹⁾ applying recursively the effective break-collapse equation (eq. 16).

For convenience, we shall introduce an energy shift in eq. (2) such that the energy between parallel spins becomes zero. We shall, thus, adopt the following form for the Hamiltonian:

$$\beta\mathcal{H}(G) = - \sum_{\epsilon \in E} \left\{ NK_{\epsilon}(\vec{S}_i \cdot \vec{S}_j - 1) + NL_{\epsilon}[(\vec{S}_i \cdot \vec{S}_j)^2 - 1] \right\} \quad (19)$$

One can rewrite eq. (10) for $D(G)$ on $Z(\lambda)$ clusters as:

$$D(G) = \frac{\lambda^{|E|-|V|}}{Az_j} Z(G) \quad (20.a)$$

where j is the chosen edge to which the effective break-collapse will be first applied and A is given by:

$$A = \prod_{\substack{\epsilon \in E \\ \epsilon \neq j}} z_{\epsilon} \quad (20.b)$$

where the above product is over all edges ϵ of E excepting j .

Combining eq. (20) with the effective break-collapse equation (16) for $D(G)(\alpha = 0)$ applied to the edge j whose vector transmissivity is $t^{(j)} = (t_1^{(j)}, t_2^{(j)})$ we obtain that

$$\frac{1}{z_1} Z(G) = \frac{t_1^{(j)}}{z_j^{cc}} Z(G_j^{cc}) + \frac{[1 - t_2^{(j)}]}{z_j^{bb}} Z(G_j^{bb}) + \frac{[t_2^{(j)} - t_1^{(j)}]}{z_j^{bc}} Z(G_j^{bc}) \quad (21)$$

where, using eq. (5), (6b), (11), (12) and (19), z_j and $z_j^{\ell m}(\ell, m = b \text{ or } c)$ are given by

$$z_j = 1 + 2(N - 1) e^{-N(K_j+L_j)} + e^{-2NK_j} \quad (22.a)$$

$$z_j^{cc} = z_j \Big|_{\substack{K \rightarrow \infty \\ L \rightarrow \infty}} = 1 \quad (22.b)$$

$$z_j^{bb} = z_j \Big|_{\substack{K \rightarrow 0 \\ L \rightarrow 0}} = 2N \quad (22.c)$$

$$z_j^{bc} = z_j \Big|_{L \rightarrow \infty} = 2 \quad (22.d)$$

The combination of eqs. (13), (21) and (22) leads to the following break-collapse equation for the partition function $Z(G)$:

$$Z(G) = p_b^{(j)} Z(G_j^{cc}) + p_r^{(j)} Z(G_j^{bc}) + p_0^{(j)} Z(G_j^{bb}) \quad (23)$$

with

$$\begin{cases} p_b^{(j)} \equiv 1 - e^{-2NK_j} & (24a) \\ p_r^{(j)} \equiv e^{-2NK_j} [1 - e^{-N(L_j-K_j)}] & (24b) \\ p_0^{(j)} \equiv 1 - (p_b^{(j)} + p_r^{(j)}) = e^{-N(K_j+L_j)} & (24c) \end{cases}$$

Notice that eq. (23) plays the same role as eq. (8) of KF⁽¹⁾. Applying recursively eq. (23) until one arrives at graphs R which are null (i.e., graphs without edges constituted exclusively by isolated vertices) and/or precollapsed, we obtain, for $p_\alpha^{(j)} \neq 0$ ($\alpha = b, r, 0$), that:

$$Z(G) = \sum_R \left[\prod_{j \in E_{cc}} p_b^{(j)} \prod_{j \in E_{bc}} p_r^{(j)} \prod_{j \in E_{bb}} p_0^{(j)} Z(R) \right] \quad (25)$$

where E_{cc} , E_{bc} and E_{bb} are the sets of edges (contained in the edge set E of G) which were respectively collapsed, precollapsed and broken in G in order to give origin to the graph R . The above sum is over all the $3^{|E|}$ graphs R generated by the application of one of these 3 operations on each edge of E . Notice that $|E_{cc}| + |E_{bc}| + |E_{bb}| = |E|$.

Let us define the graph \tilde{R} as the one obtained from R by deleting the $|V_0|$ isolated vertices such that $R = \tilde{R} \cup V_0$, where V_0 is the null graph with $|V_0|$ vertices. Thus, \tilde{R} is a precollapsed graph, and we shall denote by $E_{\tilde{R}}$ and $V_{\tilde{R}}$ its edge set and vertex set respectively. By construction, the number $w(R)$ of clusters in R is given by:

$$w(R) = w(\tilde{R}) + |V_0| \quad (26)$$

Combining eqs. (10), (22d) and (17c) one gets that:

$$Z(\tilde{R}) = (2N)^{|V_{\tilde{R}}| - |E_{\tilde{R}}|} N^{c(\tilde{R})} 2^{|E_{\tilde{R}}|} \quad (27)$$

which together with eqs. (18) and (26) leads to

$$Z(R) = (2N)^{w(R)} 2^{|E_{\bar{R}}| - c(\bar{R})} \quad (28)$$

If we add to R all the edges of E_{cc} that had been collapsed, we generate a partial² graph G' of G . Let us colour these edges, say, with blue, and the precollapsed edges, say, with red and call such graphs G' “2-coloured” *partial graphs of G* (not to be confused with bichromatic graphs since herein no constraint on the colouring is implied). Observe that the number of clusters $w(G')$ of G' is the same as that of R . But the number of cycles of only red edges in G' can be different from that of R if there are loops in R . In this case a loop of a precollapsed edge (bc) of R will become an usual red edge which belongs to a cycle with blue edges and eventually with other red edges. The number of cycles $c(R)$ of R is, thus, equal to the number of cycles formed only by red edges in G' plus the number $c^*(G')$ of independent cycles in G' which contain at least one red edge. Then, using eq. (28) we can rewrite eq. (25) as:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_r \cup G'_b}} \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_r} p_r^{(j)} \prod_{j \in E'_\phi} p_0^{(j)} \lambda^{w(G')} f(G'_r) g(G') \right\} \quad (29.a)$$

$$\text{with} \quad f(G'_r) = 2^{|E'_r| - c(G'_r)} \quad (29.b)$$

$$g(G') = 2^{-c^*(G')} \quad (29.c)$$

$$\lambda = 2N \quad (29.d)$$

where the sum is over all the $3^{|E|}$ 2-coloured partial graphs G' of G . G' is the union of the two subgraphs G'_b and G'_r with respective edge sets E'_b and E'_r which are disjoint (hence $|E'_b| + |E'_r| = |E'|$). E'_b (E'_r) is constituted of blue (red) edges, each edge j being associated with the variable $p_b^{(j)}$ ($p_r^{(j)}$). All the isolated vertices will be attributed to G'_b . The last product in E'_ϕ is over all the edges which belong to E but not to E' .

If $0 \leq K \leq L$ (which corresponds to a sub-region of the ferromagnetic case where $K \geq 0$ and $K + L \geq 0$) then $0 \leq p_\ell^{(j)} \leq 1$ ($\ell = b, r, 0$) and consequently eq. (29) can be interpreted as a polychromatic bond percolation average, namely:

$$Z(G) = \langle \lambda^w f g \rangle_{G, p_b, p_r} \quad (30)$$

where $\langle \dots \rangle_{G, p_b, p_r}$ stands for an average over all the bond configurations in a polychromatic bond percolation problem⁽²⁷⁾ with 2 types of present bonds on the graph G , where the

²A partial graph G' of G is a subgraph of G which has the same vertex set as that of G , i.e., $V' = V$ and $E' \subseteq E$.

blue bonds (b) and the red bonds (r) occur with independent respective probabilities $p_b^{(j)}$ and $p_r^{(j)}$ (which are related to K_j and L_j through eqs. (24a) and (24b)).

Now let us focus on the correlation functions. Let us define $\Gamma_1(1, 2; G)$ and $\Gamma_2(1, 2; G)$ by:

$$\Gamma_1(1, 2; G) \equiv \sum_{\{\vec{S}_i\}} \left\{ e^{-\beta\mathcal{H}(G)} \vec{S}_1 \cdot \vec{S}_2 \right\} \quad (31)$$

and

$$\Gamma_2(1, 2; G) \equiv \sum_{\{\vec{S}_i\}} \left\{ e^{-\beta\mathcal{H}(G)} \left[\frac{N(\vec{S}_1 \cdot \vec{S}_2)^2 - 1}{N - 1} \right] \right\} \quad (32)$$

where the sum is over all possible configurations of the spins $\{\vec{S}_i\}$ ($i = 1, 2, \dots, |V|$).

Combining eqs. (9), (14), (15), (31) and (32) one gets that:

$$\Gamma_\alpha(1, 2; G) = Z(G)T_\alpha(1, 2; G) = \sum_{\{n_i\}} e^{-2\pi i\alpha(n_1 - n_2)/\lambda} \prod_{e \in E} e^{-h_e(n_i - n_j)} \quad (33)$$

$(\alpha = 1, 2)$

Using the results of⁽³¹⁾ (see their eqs. (2.16), (2.17) and (2.18)) one can show that:

$$\Gamma_\alpha(1, 2; G) = \lambda^{|V| - |E|} \left(\prod_{e \in E} z_e \right) N_\alpha(1, 2; G) \quad (34)$$

$(\alpha = 1, 2)$

which is similar to eq. (10) that relates $Z(G)$ with $D(G)$. Repeating the same procedure used for deriving eq. (23) from eq. (10), we obtain that:

$$\Gamma_\alpha(1, 2; G) = p_b^{(j)} \Gamma_\alpha(1, 2; G_j^{cc}) + p_r^{(j)} \Gamma_\alpha(1, 2; G_j^{bc}) + p_0^{(j)} \Gamma_\alpha(1, 2; G_j^{bb}) \quad (35)$$

$(\alpha = 1, 2)$

Applying recursively eq. (35) for $\alpha = 2$ and using eqs. (17b), (18), (22d), (26) and (34) one gets, similarly to the expression (29), that:

$$\Gamma_2(1, 2; G) = \sum_{\substack{G' \subseteq G \\ G' = G'_r \cup G'_b}} \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_r} p_r^{(j)} \prod_{j \in E'_\phi} p_0^{(j)} \lambda^{w(G')} \gamma_{12}^{(G\ell)}(G') f(G'_r) g(G') \right\} \quad (36)$$

where the superscript $(G\ell)$ stands for global since both blue and red edges can contribute for a path between 1 and 2. Eq. (36), for $0 < K \leq L$, can be written as a polychromatic bond percolation average, namely:

$$\Gamma_2(1, 2; G) = \langle \lambda^w f g \gamma_{12}^{(G\ell)} \rangle_{G, p_b, p_r} \quad (37)$$

Concerning the other correlation function $\Gamma_1(1, 2; G)$, due to its special property (17a), one has to apply eq. (35) iteratively until one arrives at graphs which contain isolated vertices, only *one* root, and edges which are all precollapsed ones, except the eventual loops of collapsed edges. This unique root arises from the collapse of the two roots, which will give origin to a factor $\gamma_{12}(G'_b)$ after adding the previously collapsed (blue) edges. Similarly, to eq. (29a) one gets that:

$$\Gamma_1(1, 2; G) = \sum_{\substack{G' \subseteq G \\ G' = G'_r \cup G'_b}} \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_r} p_r^{(j)} \prod_{j \in E'_\phi} p_0^{(j)} \lambda^{w(G')} \gamma_{12}^{(b)}(G'_b) f(G'_r) g(G') \right\} \quad (38)$$

which, for $0 < K \leq L$, leads to

$$\Gamma_1(1, 2; G) = \langle \lambda^w f g \gamma_{12}^{(b)} \rangle_{G, p_b, p_r} \quad (39)$$

where the superscript b stands for blue since there must be, at least, one path of *solely* blue bonds connecting 1 and 2 in order that $\gamma_{12}^{(b)}(G'_b) = 1$ (otherwise $\gamma_{12}^{(b)}(G'_b) = 0$).

It is worth stressing that alternative polychromatic bond percolation average forms for $D(G)$, $N_1(1, 2, G)$ and $N_2(1, 2, G)$ have been obtained by Arrowsmith and Essam⁽¹⁴⁾. Their averages are expressed in variables different from our $p_b^{(j)}$ and $p_r^{(j)}$ ones, the quantities to be averaged have no simple formulae and no relations are given between the thermal properties and the geometrical ones in the $\lambda \rightarrow 1$ limit.

4 The $\lambda \rightarrow 1$ limit case: A new kind of percolation problem

4.1 General Results

In the previous formulation it appeared a factor fg in the percolation averages which prevents us to accomplish the second step mentioned in section 1, i.e., we failed to relate the thermal properties of the cubic model with the geometric ones of the polychromatic bond percolation problem when the number of states $\lambda = 2N$ tends to 1. In this section we shall present a two-step geometrical formulation in which this is possible provided that certain bond configurations are avoided, similar to what happens in the bond frustrated percolation (BFP) problem^(12,13).

The central point for obtaining this new formulation consists in noticing that in one precollapsed edge e^{bc} (characterized by $K_e = 0$ and $L_e \rightarrow \infty$), which links the vertices i

and j , the spins \vec{S}_i and \vec{S}_j must be such that $(\vec{S}_i \cdot \vec{S}_j)^2 = 1$ (see eq. 19), i.e. $\vec{S}_i = \pm \vec{S}_j$. Therefore one can split its partition function $Z(e^{bc})$ into two parts: one corresponding to $\vec{S}_i = \vec{S}_j$ (becoming a collapsed edge) and the other to the case where $\vec{S}_i = -\vec{S}_j$ (generating what we shall call an “*anti-collapsed*” edge e^{ac}), namely:

$$Z(e^{bc}) = Z(e^{cc}) + Z(e^{ac}) \quad (40)$$

Therefore one can generate $2^{|E_{\tilde{R}}|}$ graphs from a precollapsed graph \tilde{R} (defined in the previous section) by attributing to each of its $|E_{\tilde{R}}|$ precollapsed edges one of the two possibilities: either an yellow edge (corresponding to the condition $S_i = S_j$ of a collapsed edge) or a green edge (corresponding to the condition $S_i = -S_j$ of an anti-collapsed edge). Then, one can show (see the proof in the Appendix) that from these $2^{|E_{\tilde{R}}|}$ graphs only $f(\tilde{R}) = 2^{|E_{\tilde{R}}| - c(\tilde{R})}$ graphs do not contain any cycle with an odd number of green edges. Let us denote by \tilde{R}_{nf} each of such graphs (the subscript nf stands for non-frustrated for reasons which will become clear later on). Notice that the other graphs (i.e., the “frustrated” ones) do not contribute for $Z(\tilde{R})$, and hence:

$$Z(\tilde{R}) = \sum_{\tilde{R}_{nf}} Z(\tilde{R}_{nf}) \quad (41)$$

If the state of \vec{S}_i located on one of the vertices of a cluster of a given \tilde{R}_{nf} is fixed, then, the states of the spins on the other vertices of this cluster become automatically determined without any incompatibility. Therefore its partition function is given by

$$Z(\tilde{R}_{nf}) = (2N)^{w(\tilde{R}_{nf})} \quad (\forall \tilde{R}_{nf}) \quad (42)$$

Observe that in the generation of \tilde{R}_{nf} from \tilde{R} there is no alteration in the number of clusters, i.e.

$$w(\tilde{R}_{nf}) = w(\tilde{R}) \quad (43)$$

Combining this eq. with the previous results, one obtains that

$$Z(\tilde{R}) = (2N)^{w(\tilde{R})} 2^{|E_{\tilde{R}}| - c(\tilde{R})} \quad (44)$$

Adding thus the $|V_0|$ isolated vertices to \tilde{R} in order to form R , and using eq. (26), one finally arrives to eq. (28). If one attributes a zero weight to the frustrated graphs R_f (i.e., $Z(R_f) = 0$), then this shows that the replacement of each graph R by the $2^{|E_R|}$ new graphs (where each of its red edges have been substituted, say, by either an yellow or green edge) does not alter the original partition function $Z(R)$ of the graph R . Now, let us

add all the edges $e \in E_{cc}$ of G which had been collapsed during the process of generating R , and colour them with blue. If one considers all the $3^{|E|}$ original bond configurations (where each edge can be blue, red or absent) and then replace each red edge by either, say, a green or yellow one, it will be generated, at the end, $4^{|E|}$ bond configurations where each edge can be blue, green, yellow or absent. This can be easily seen if one considers all the combinations of $|E|$ with ℓ ($\ell = 0, 1, \dots, |E|$) red bonds giving $3^{|E|} = \sum_{\ell=0}^{|E|} C_\ell^{|E|} 2^{|E|-\ell}$ configurations and, after substitution of the red edges by the green and yellow bonds, one obtains $\sum_{\ell=0}^{|E|} C_\ell^{|E|} 2^{|E|-\ell} = 2^{|E|} \sum_{\ell=0}^{|E|} C_\ell^{|E|} = 4^{|E|}$ configurations. From these $4^{|E|}$ possibilities (which constitute all the “3-coloured” partial graphs G' of G), only those in which each cycle has an even number of green edges contribute to the partition function $Z(G)$.

Taking into account all the above considerations, one can rewrite eq. (25) as:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}} \star \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_{gr}} p_{gr}^{(j)} \prod_{j \in E'_y} p_y^{(j)} \prod_{j \in E'_\phi} p_0^{(j)} \lambda^{w(G')} \right\} \quad (45.a)$$

with

$$p_{gr}^{(j)} = p_y^{(j)} = p_r^{(j)} \quad (45.b)$$

where the star means that the sum in the “3-coloured” partial graphs G' of G must be taken only over those configurations in which each cycle has an even number of green bonds. G' is the union of the three subgraphs G'_b , G'_{gr} and G'_y with respective disjoint edge sets E'_b (with blue edges), E'_{gr} (with green edges) and E'_y (with yellow edges). Observe that $|E'_b| + |E'_{gr}| + |E'_y| = |E'|$, and that the last product is over the absent edges E'_ϕ (they belong to E but not to $E' = E'_b \cup E'_{gr} \cup E'_y$). Notice that with each type α of edge j ($\alpha = \text{Blue } (b), \text{ green } (gr) \text{ or yellow } (y)$) is associated a weight $p_\alpha^{(j)}$, but an absent edge j is associated with a weight $p_0^{(j)} = 1 - (p_b^{(j)} + p_r^{(j)})$ which is different from the complement of the others (i.e., $p_0^{(j)} \neq 1 - (p_b^{(j)} + p_y^{(j)} + p_{gr}^{(j)})$). This inconvenience can be overcome by dividing and multiplying eq. (45a) by the factor $\prod_{j=1}^{|E|} (p_b^{(j)} + p_{gr}^{(j)} + p_y^{(j)} + p_0^{(j)})$ and using that

$$|E| = |E'_b| + |E'_{gr}| + |E'_y| + |E'_\phi| \quad (46)$$

One can, thus, rewrite eq. (45a) as:

$$Z(G) = \prod_{j=1}^{|E|} (p_b^{(j)} + p_{gr}^{(j)} + p_y^{(j)} + p_0^{(j)}) \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}} \star \left\{ \prod_{j \in E'_b} \alpha_b^{(j)} \prod_{j \in E'_{gr}} \alpha_{gr}^{(j)} \prod_{j \in E'_y} \alpha_y^{(j)} \prod_{j \in E'_\phi} \alpha_0^{(j)} \lambda^{w(G')} \right\} \quad (47)$$

with

$$\alpha_\ell^{(j)} \equiv \frac{p_\ell^{(j)}}{p_b^{(j)} + p_{gr}^{(j)} + p_y^{(j)} + p_0^{(j)}} \quad (\ell = b, gr, y \text{ or } 0 \text{ (absent)}) \quad (48)$$

which are given in terms of K and L as (see definitions (24)):

$$\alpha_b^{(j)} = \frac{1 - e^{-2NK_j}}{1 + e^{-2NK_j} - e^{-N(K_j+L_j)}} \quad (49.a)$$

$$\alpha_{gr}^{(j)} = \alpha_y^{(j)} = \frac{e^{-2NK_j} - e^{-N(K_j+L_j)}}{1 + e^{-2NK_j} - e^{-N(K_j+L_j)}} \quad (49.b)$$

and

$$\alpha_0^{(j)} = 1 - (\alpha_b^{(j)} + \alpha_{gr}^{(j)} + \alpha_y^{(j)}) = \frac{e^{-N(K_j+L_j)}}{1 + e^{-2NK_j} - e^{-N(K_j+L_j)}} \quad (49.c)$$

When $0 \leq K \leq L$ then $0 \leq \alpha_\ell^{(j)} \leq 1$ ($\ell = b, gr, y$ or 0) and we can write eq. (47) as the following special percolation (SP) type average:

$$Z(G) = A(\{K_j\}, \{L_j\}) \langle \lambda^w \rangle_{G,SP} \quad (50)$$

with

$$A(\{K_j\}, \{L_j\}) = \prod_{j=1}^{|E|} [1 + e^{-2NK_j} - e^{-N(K_j+L_j)}] \quad (51)$$

$\langle \dots \rangle_{G,SP}$ stands for an average over all the bond configurations in a new kind of polychromatic bond percolation problem in which there are 3 types of present edges $\{j\}$ (say, the blue (b), the yellow (y), and the green (gr) ones) on the graph G with the constraint that each cycle of a configuration contains *only an even number of green edges*. Each edge j ($j = 1, 2, \dots, |E|$) has probabilities $\alpha_b^{(j)}$, $\alpha_y^{(j)}$, $\alpha_{gr}^{(j)} = \alpha_y^{(j)}$ and $1 - (\alpha_b^{(j)} + \alpha_y^{(j)} + \alpha_{gr}^{(j)})$ (defined in eq. (49)) of being blue, yellow, green or absent, respectively. Notice that if we associate with a green edge j a value $\varepsilon_j = -1$ (playing the role similar to that of an antiferromagnetic AF bond) and if we associate the value $\varepsilon_j = +1$ (playing the role similar to that of a ferromagnet F bond) with a blue or yellow edge j , then the only allowed configurations are those which are *not frustrated*. In other words, the frustrated cycles ℓ_f , characterized by

$$\ell_f = \prod_{j \in \ell_f} \varepsilon_j = -1 \quad (52)$$

are forbidden in the above percolation problem and, within the above convention, the symbol star can be interpreted as a sum over configurations of positive and negative bonds which do not contain any frustrated cycle. A similar fact occurs in the BFP model^(12,13) which is related to spin glasses and glasses. But in the BFP, the lattice

(or any graph G) is first prepared by randomly assigning to each edge j the variable $\varepsilon_j = \pm 1$ with *equal probabilities* and, only after fixing the distribution of $\{\varepsilon_j\}$, the bonds are randomly introduced onto the edges (regardless of the sign of ε_j) with the constraint of not giving origin to any frustrated cycle. This procedure generates, at each time the bonds are thrown without frustration, a “2-coloured” partial graph G' of G whose edges are positive, negative (with equiprobability) or absent and such that each cycle has an even number of negative bonds. Therefore, the set $\phi(G, \{\varepsilon_j\})$ of all possible bond configurations $G' \subseteq G$ with no frustration which appear in the BFP problem contains only configurations compatible with a given distribution of $\{\varepsilon_j\}$, constituting thus only a *subset* of the set $\phi(G)$ of all non-frustrated configurations of G . Furthermore, the union of the sets $\phi(G, \{\varepsilon_j\})$ over all the possible distributions $\{\varepsilon_j\}$ is different from $\phi(G)$ since there are bond configurations compatible with distinct distributions $\{\varepsilon_j\}$. This is the reason why our percolation problem does not reduce, for $\alpha_b^{(j)} = 0$ (where the positive and negative bonds become equiprobable), to the BFP model. In a similar way, our result eq. (50) does not recover, for $\alpha_b^{(j)} = 0$, that of Coniglio⁽¹³⁾ for the partition function of the frustrated q -state Potts model (with $q = 2N$).

Following a procedure similar to the one used for deducing eq. (50), we can derive from eq. (35) the following eqs. for $\Gamma_\alpha(1, 2; G)(\alpha = 1, 2)$:

$$\begin{aligned} \Gamma_2(1, 2; G) &= A(\{K_j\}, \{L_j\}) \times \\ &\times \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}}^* \left\{ \prod_{j \in E'_b} \alpha_b^{(j)} \prod_{j \in E'_{gr}} \alpha_{gr}^{(j)} \prod_{j \in E'_y} \alpha_y^{(j)} \prod_{j \in E'_\phi} \alpha_0^{(j)} \lambda^{w(G')} \gamma_{12}^{(G\ell)}(G') \right\} \end{aligned} \quad (53)$$

and

$$\begin{aligned} \Gamma_1(1, 2; G) &= A(\{K_j\}, \{L_j\}) \times \\ &\times \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}}^* \left\{ \prod_{j \in E'_b} \alpha_b^{(j)} \prod_{j \in E'_{gr}} \alpha_{gr}^{(j)} \prod_{j \in E'_y} \alpha_y^{(j)} \prod_{j \in E'_\phi} \alpha_0^{(j)} \lambda^{w(G')} \gamma_{12}^{(b)}(G'_b) \right\} \end{aligned} \quad (54)$$

which can be rewritten, for $0 \leq K \leq L$, as the respective special percolation averages:

$$\Gamma_2(1, 2; G) = A(\{K_j\}, \{L_j\}) \langle \lambda^w \gamma_{12}^{(G\ell)} \rangle_{G,SP} \quad (55)$$

and

$$\Gamma_1(1, 2; G) = A(\{K_j\}, \{L_j\}) \langle \lambda^w \gamma_{12}^{(b)} \rangle_{G,SP} \quad (56)$$

Following along the lines of Wu⁽⁵⁾, we can now accomplish the mentioned second step of our formulation, establishing the relations in the $\lambda \rightarrow 1$ limit, between $Z(G)$ (eq. 50),

$\Gamma_2(1, 2; G)$ (eq. 55), $\Gamma_1(1, 2; G)$ (eq. 56) and respective characteristic quantities of the above special percolation, namely:

i) the mean number of clusters per site $n(G)$

$$n(G) \equiv \lim_{|V| \rightarrow \infty} \frac{1}{|V|} \langle w \rangle_{G,SP} = \lim_{\lambda \rightarrow 1} \frac{\partial F(G)}{\partial \lambda} \quad (57.a)$$

where $F(G)$ is proportional to the free energy per site given by

$$F(G) = \lim_{|V| \rightarrow \infty} \frac{1}{|V|} \ln \left[\frac{Z(G)}{A(\{K_j\}, \{L_j\})} \right] \quad (57.b)$$

ii) the global pair connectedness $C_{12}^{(G\ell)}(G)$, i.e., the probability that the sites 1 and 2 are connected through any types of edges

$$C_{12}^{(G\ell)}(G) \equiv \langle \gamma_{12}^{(G\ell)} \rangle_{G,SP} = \lim_{\lambda \rightarrow 1} \frac{\partial \tilde{\Gamma}_2(1, 2; G)}{\partial \lambda} \quad (58.a)$$

where $\tilde{\Gamma}_2(1, 2; G)$ is proportional to a pair correlation function given by

$$\tilde{\Gamma}_2(1, 2; G) = \frac{(2N - 1)}{(2N)^2} T_2(1, 2; G) \quad (58.b)$$

with $T_2(1, 2; G)$ being defined by eq. (15) (see also eq. 33)

iii) the blue pair connectedness $C_{12}^{(b)}(G)$, i.e., the probability that the sites 1 and 2 are connected through exclusively *blue* bonds:

$$C_{12}^{(b)}(G) \equiv \langle \gamma_{12}^{(b)} \rangle_{G,SP} = \lim_{\lambda \rightarrow 1} \frac{\partial \tilde{\Gamma}_1(1, 2; G)}{\partial \lambda} \quad (59.a)$$

where $\tilde{\Gamma}_1(1, 2; G)$ is proportional to the other pair correlation function, namely:

$$\tilde{\Gamma}_1(1, 2; G) = \frac{(2N - 1)}{(2N)^2} T_1(1, 2; G) \quad (59.b)$$

with $T_1(1, 2; G)$ being defined by eq. (14) (see also eq. 33).

4.2 Particular Cases

Now let us show that our general expressions eqs. (50), (55) and (56) reproduce correctly the expected results in different particular cases of the cubic model.

i) $K_j = 0$

Our Hamiltonian (eq. 19) reduces, for $K_j = 0$, to that of a N -state Potts model (with coupling constant NL_j) together with $|V|$ independent $S = 1/2$ spins. In this case, the probabilities $\alpha_\ell^{(j)}$ (eqs. 49) become:

$$\alpha_b^{(j)} = 0 \tag{60.a}$$

$$\alpha_{gr}^{(j)} = \alpha_y^{(j)} = \frac{1 - e^{-NL_j}}{2 - e^{-NL_j}} \tag{60.b}$$

and

$$\alpha_0^{(j)} = 1 - (\alpha_{gr}^{(j)} + \alpha_y^{(j)}) = \frac{e^{-NL_j}}{2 - e^{-NL_j}} \tag{60.c}$$

and the factor $A(\{K_j\}, \{L_j\})$ (eq. 51) becomes

$$A(K_j = 0, \{L_j\}) = \prod_{j=1}^{|E|} (2 - e^{-NL_j}) \tag{61}$$

The vanishment of $\alpha_b^{(j)}$ does not imply that $Z(G) = 0$ since eq. (50) was derived by the recursive application of eq. (23) assuming that each of its three terms is non null. In the case $K_e = 0$, the collapsed graphs do not contribute to $Z(G)$ since $p_b^{(j)}$ vanishes. In this situation, the iteration of eq. (23) leads to a modification of eq. (25), namely, the absence of the product of $p_b^{(j)}$ over the collapsed edges E_{cc} . Consequently, the product of $\alpha_b^{(j)}$ over the blue edges contained in the definition of the special percolation type average (see eq. 47) disappears and all the subgraphs G'_b are null ones. Taking this into account and combining eqs. (60), (61) and (50), the partition function becomes:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}} \star \prod_{\substack{j \in E' \\ (E' = E'_{gr} \cup E'_y)}} p^{(j)} \prod_{j \in E'_\phi} (1 - p^{(j)}) \lambda^{w(G')} \tag{62.a}$$

with

$$p^{(j)} = 1 - e^{-NL_j} \tag{62.b}$$

Notice that $p^{(j)}$ is equal to the probability of a red edge $p_r^{(j)}$ when $K_j = 0$ (see eq. 24b). If we invert the reasoning which led us to derive eq. (50) from eq. (29), i.e., if we think that a green or yellow edge was originated by a red one and remember that from the $2^{|E'|}$ possible graphs with $|E'|$ red edges (notice that $|E'| = |E'_r|$ since $|E'_b| = 0$) only $2^{|E'| - c(G')}$ graphs are not frustrated, then we get that:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_r \cup G'_b}} \prod_{\substack{j \in E'_\phi \\ (E' = E'_r)}} p^{(j)} \prod_{j \in E'_\phi} (1 - p^{(j)}) \lambda^{w(G')} 2^{|E'| - c(G')} \tag{63}$$

which is equal to eq. (29a) specialized to the case where there are no blue edges (since the first product of eq. (29a) would be absent when $p_b^{(j)} = 0$ for the reasons explained above).

Using the Euler relation (eq. 18) and incorporating all the isolated vertices (which belong to G'_b) to G'_r such that $G' = G'_r$ (and, hence, $|V'| = |V|$) we, finally, arrive at

$$Z(G) = 2^{|V|} \sum_{G' \subseteq G} \prod_{j \in E'} p^{(j)} \prod_{j \in E'_\phi} (1 - p^{(j)}) N^{w(G')} \quad (64)$$

or, equivalently,

$$Z(G) = 2^{|V|} Z_{KF}(G) \quad (65.a)$$

with

$$Z_{KF}(G) = \langle N^w \rangle_{G,p^{(j)}} \quad (65.b)$$

where $\langle \dots \rangle_{G,p^{(j)}}$ stands for the usual bond percolation average on a graph G in which the occupancy probability of an edge j is $p^{(j)}$ defined in eq. (62b). $Z_{KF}(G)$ is the result obtained by $\text{KF}^{(1)}$ for the q -state ($q = N$) Potts model described by the dimensionless Hamiltonian

$$\beta \mathcal{H}_{KF}(G) = - \sum_{e \in E} q L_e [\delta(\sigma_i, \sigma_j) - 1] \quad (\sigma_i = 1, 2, \dots, q) \quad (66)$$

where σ_i is the Potts variable associated with each vertex i of G and $\delta(\sigma_i, \sigma_j)$ is the Kronecker function.

Therefore, our result eq. (65) corresponds to the partition function of the N -state Potts model (with coupling constant NL_e) and $|V|$ independent $S = 1/2$ spins (the latter has $2^{|V|}$ configurations with zero energy leading, thus, to the factor $2^{|V|}$ in eq. (65a)), recovering the expected results for $K_j = 0$.

Similarly, we obtain that $\Gamma_2(1, 2; G)$, (eq. 55) reduces, for $K_j = 0$, to:

$$\Gamma_2(1, 2; G) = 2^{|V|} \Gamma_{KF}(1, 2; G) \quad (67.a)$$

with

$$\Gamma_{KF}(1, 2; G) = \langle N^w \gamma_{12} \rangle_{G,p^{(j)}} \quad (67.b)$$

where, again, $\Gamma_{KF}(1, 2; G)$ is the result obtained by $\text{KF}^{(1)}$ for the N -state Potts model in what concerns the correlation function $\Gamma_{12}(G)$, i.e.

$$\Gamma_{KF}(1, 2; G) = Z(G) \Gamma_{12}(G) = Z(G) \overline{\left(\frac{q \delta(\alpha_1, \alpha_2) - 1}{q - 1} \right)} \quad (68)$$

The factor $2^{|V|}$ in eq. (67a) comes from the $|V|$ independent $S = 1/2$ spins and we get, again, the recovering of the expected results for $K_j = 0$.

Concerning $\Gamma_1(1, 2; G)$ (eq. 56), it vanishes when $K_j = 0$ due to the absence of blue edges (since in that case $\gamma_{12}^{(b)}(G'_b) = 0$). This is in agreement with the fact that $N_1(1, 2; G)$ becomes null whenever $K_j = 0^{(24)}$, which renders $\Gamma_1(1, 2; G) = 0$ (cf eq. (34)).

ii) $K_j = L_j$

When $K_j = L_j$ the studied model reduces to a $2N$ -state Potts model with coupling constant $2NK_j$. In this situation $\alpha_\ell^{(j)}$ (eqs. 49) become

$$\alpha_b^{(j)} = 1 - e^{-2NK_j} \tag{69.a}$$

$$\alpha_{gr}^{(j)} = \alpha_y^{(j)} = 0 \tag{69.b}$$

and

$$\alpha_0^{(j)} = 1 - \alpha_b^{(j)} = e^{-2NK_j} \tag{69.c}$$

while $A(\{K_j\}, \{L_j\})$ (eq. 51) reduces to

$$A(\{K_j = L_j\}) = 1 \tag{70}$$

The vanishment of $\alpha_{gr}^{(j)}$ and $\alpha_y^{(j)}$ implies that $p_r^{(j)} = 0$ (cf eq. 48) and, therefore, the precollapsed edges do not contribute to $Z(G)$. The iteration of eq. (23) for $p_r^{(j)} = 0$ would lead, at the end, to a special percolation type average (eq. 47) without the products of $\alpha_{gr}^{(j)}$ and $\alpha_y^{(j)}$ over the respective green and yellow edges. Furthermore, the restriction of summing only on subgraphs with an even number of green edges becomes uneffective (as there are no green edges) and the star sum equals the usual one over all the subgraphs G' (whose edges are all blue, i.e., $G' = G'_b$) of G . Eqs. (50), (55) and (56) reduce in this case to:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_b}} \prod_{j \in E'} \alpha_b^{(j)} \prod_{j \in E'_\phi} (1 - \alpha_b^{(j)}) \lambda^{w(G')} = \langle \lambda^w \rangle_{G, p^{(j)} = \alpha_b^{(j)}} \tag{71}$$

and

$$\Gamma_2(1, 2; G) = \Gamma_1(1, 2; G) = \langle \lambda^w \gamma_{12} \rangle_{G, p^{(j)} = \alpha_b^{(j)}} \tag{72}$$

which recover the expected results⁽¹⁾ for the λ -state Potts model with coupling constant $2NK_j$. Combining eqs. (34) and (72) we obtain that $N_1(1, 2; G) = N_2(1, 2; G)$ as it should be⁽²⁴⁾.

iii) $L_j/|K_j| \rightarrow \infty$

The case $L_j/|K_j| \rightarrow \infty$ corresponds to N decoupled Ising models, each of which has coupling constant NK_j . In this situation eqs. (49) and (51) reduce to

$$\alpha_b^{(j)} = \frac{1 - e^{-2NK_j}}{1 + e^{-2NK_j}} \quad (73.a)$$

$$\alpha_{gr}^{(j)} = \alpha_y^{(j)} = \frac{e^{-2NK_j}}{1 + e^{-2NK_j}} = 1 - \alpha_b^{(j)} \quad (73.b)$$

$$\alpha_0^{(j)} = 0 \quad (73.c)$$

and

$$A(\{K_j\}, \{L_j \rightarrow \infty\}) = \prod_{j=1}^{|E|} (1 + e^{-2NK_j}) \quad (74)$$

The vanishment of $\alpha_0^{(j)}$ and, consequently, of $p_0^{(j)}$ (cf eq. (48)) indicates that there are no absent edges. Therefore the broken edges do not contribute, in this case, to the partition function, and the iteration of eq. (23) for $p_0^{(j)} = 0$ would lead, at the end, to an SP average without the product in $\alpha_0^{(j)}$. Eq. (50) becomes, after using eqs. (73) and (74):

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_{gr} \cup G'_y}}^* \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_{gr} \cup E'_y} (1 - p_b^{(j)}) \lambda^{w(G')} \right\} \quad (75)$$

where $p_b^{(j)}$ is the occupancy probability of a blue edge j defined in eq. (24a). Similarly to the particular case (i), we can replace the green and yellow edges by red ones, transforming the above star sum into an usual one, namely:

$$Z(G) = \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_r}} \left\{ \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_r} (1 - p_b^{(j)}) \lambda^{w(G')} 2^{|E'_r| - c(G'_r) - c^*(G')} \right\} \quad (76)$$

Due to the lack of absent edges it follows that:

$$w(G') = w(G) \quad (77.a)$$

and

$$|E'_r| + |E'_b| = |E| \quad (77.b)$$

and using the Euler relation eq. (18), we can rewrite eq. (76) as:

$$Z(G) = N^{w(G)} \sum_{\substack{G' \subseteq G \\ G' = G'_b \cup G'_r}} \prod_{j \in E'_b} p_b^{(j)} \prod_{j \in E'_r} (1 - p_b^{(j)}) 2^{|V| - |E'_b| + c(G) - c(G'_r) - c^*(G')} \quad (78)$$

Constructing graphs G'' by deleting the red edges of G' , it follows that all the edges of the edge set E'' of G'' are blue and that:

$$|V| = |V''| \tag{79.a}$$

$$|E'_b| = |E''| \tag{79.b}$$

and

$$c(G'') = c(G) - [c(G'_r) + c^*(G')] \tag{79.c}$$

The combination of eqs. (18), (78) and (79) leads, finally, to:

$$Z(G) = N^{w(G)} \sum_{G'' \subseteq G} \prod_{j \in E''} p_b^{(j)} \prod_{j \in E''_\phi} (1 - p_b^{(j)}) 2^{w(G'')} = N^{w(G)} Z_{KF}^{Is}(G) \tag{80}$$

where $Z_{KF}^{Is}(G)$ is the $KF^{(1)}$ result for the Ising model with coupling constant NK_j . Our result eq. (80) corresponds, thus, to N decoupled Ising models, recovering the appropriate one.

Concerning the function $\Gamma_2(1, 2; G)$ (eq. (55) since, in the considered situation, there are no absent edges, then the following equality holds:

$$\gamma_{12}^{G\ell}(G') = \gamma_{12}^{G\ell}(G) \tag{81}$$

which would lead to a result similar to eq. (80), namely

$$\Gamma_2(1, 2; G) = N^{w(G)} \gamma_{12}(G) Z_{KF}^{Is}(G) \tag{82}$$

and, consequently (cf eq. (33)),

$$T_2(1, 2; G) = \gamma_{12}(G) \tag{83}$$

Although, in this case, $\Gamma_2(1, 2; G)$ does not provide any useful information about the correlation function, this does not occur with $\Gamma_1(1, 2; G)$ (eq. 56). Following the previous procedure, we would arrive at an equation similar to eq. (78) except by the additional factor $\gamma_{12}^{(b)}(G'_b)$ which becomes, after the deletion of the red edges, identical to $\gamma_{12}(G'')$. Hence we get that:

$$\Gamma_1(1, 2; G) = N^{w(G)} \sum_{G'' \subseteq G} \prod_{j \in E''} p_b^{(j)} \prod_{j \in E''_\phi} (1 - p_b^{(j)}) 2^{w(G'')} \gamma_{12}(G'') = N^{w(G)} \langle 2^w \gamma_{12} \rangle_{G, p_b^{(j)}} \tag{84}$$

which, combined with eqs. (33) and (80), leads to the expected result, namely:

$$T_1(1, 2; G) = \frac{\langle 2^w \gamma_{12} \rangle_{G, p_b^{(j)}}}{\langle 2^w \rangle_{G, p_b^{(j)}}} = \Gamma_{12}^{Is}(G)$$

where $\Gamma_{12}^{Is}(G)$ is the correlation function of the Ising model with coupling constant $NK_j^{(1)}$.

iv) $N = 1$ (Ising Model)

In the $N = 1$ case, which corresponds to the Ising Model, it has been shown⁽²⁴⁾ that the vector transmissivity has only one component ($\vec{t}_e = t_e(1) = tghK_e$) and that

$$D(G_j^{bc}) = D(G_j^{bb}) \quad (85.a)$$

and

$$N_1(G_j^{bc}) = N_1(G_j^{bb}) \quad (85.b)$$

Combining the above equations with eqs. (20)-(22) we obtain, instead of eq. (23), the following break-collapse equation for $Z(G)$ when $N = 1$:

$$Z(G) = p_b^{(j)} Z(G_j^{cc}) + (1 - p_b^{(j)}) Z(G_j^{bb}) \quad (86.a)$$

with

$$p_b^{(j)} = 1 - e^{-2K_j} = 1 - (p_r^{(j)} + p_0^{(j)}) \quad (86.b)$$

which coincides with eq. (8) of⁽¹⁾. Since there are no broken-collapsed edges and, therefore, no green and yellow edges, eqs. (50) and (56) would reduce, similarly to the particular case (ii), to:

$$Z(G) = \langle 2^w \rangle_{G, p_b^{(j)}} \quad (87.a)$$

and

$$\Gamma_1(1, 2; G) = \langle 2^w \gamma_{12} \rangle_{G, p_b^{(j)}} \quad (87.b)$$

which recover the KF results⁽¹⁾ for the Ising model with coupling constant K_j , as it should be.

5 Conclusions

We prove, herein, that the discrete N -component cubic model is related, in the $\lambda = 2N \rightarrow 1$ limit, to a new kind of percolation problem in the same way as standard bond percolation is connected to the $q \rightarrow 1$ limit of the Potts model. Despite this relation occurs only for the ferromagnetic case of the cubic model, this new percolation can be regarded as one in which there are negative bonds and two types of positive bonds subjected to the constraint that the only allowed configurations are those without frustration. Although

this restriction appears also in the bond-frustrated percolation, which was introduced⁽¹²⁾ in the context of spin glasses and glasses, our percolation problem is essentially different from it (where a further restriction of the quenched type on the allowed configurations is imposed).

We hope that, as the Kasteleyn and Fortuin⁽¹⁾ percolation formulation was successfully used by Swendsen and Wang⁽¹⁶⁾ in the construction of a cluster Monte Carlo algorithm for the Potts ferromagnet, our results are used for the development of a *cluster* dynamics which would considerably reduce the critical slowing down in Monte Carlo simulations of the cubic model. Work along this line is in progress.

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Appendix

Proof of the equality $f(\tilde{R}) = 2^{|E_{\tilde{R}}|-c(\tilde{R})}$

In this appendix we prove that, from the $2^{|E_{\tilde{R}}|}$ graphs generated from a connected precollapsed graph \tilde{R} by attributing to each of its $|E_{\tilde{R}}|$ edges either an yellow or a green color, only $f(\tilde{R})$ graphs do not contain any cycle with an odd number of green edges.

Let us consider a fundamental cycle basis constituted by the independent cycle vectors $\vec{\mu}^{(1)}, \vec{\mu}^{(2)}, \dots, \vec{\mu}^{(c)}$ associated with some spanning tree⁽³⁴⁾ of the graph \tilde{R} (whose cyclomatic number $c(\tilde{R})$ we shall simply denote by c). $\vec{\mu}^{(i)}$ is an $|E_{\tilde{R}}|$ -dimensional vector whose components $\mu_{\alpha}^{(i)}$ ($\alpha = 1, 2, \dots, |E_{\tilde{R}}|$) are 1 or 0 depending if the edge e_{α} belongs or not, respectively, to the cycle $\mu^{(i)}$ ($i = 1, 2, \dots, c$). Let us denote by k_i the number of edges that belong *exclusively* to the cycle $\mu^{(i)}$ (notice that $k_i \neq 0 \forall i$ for any basis associated with a spanning tree). Since every edge of \tilde{R} must belong to one of the c independent cycles, it follows that

$$k + \ell = |E_{\tilde{R}}| \tag{1.a}$$

with

$$k = \sum_{i=1}^c k_i \tag{1.b}$$

where $\ell \geq 0$ is the number of edges of \tilde{R} which belong to two or more cycles $\mu^{(i)}$. We shall denote these edges by $a_1, a_2, \dots, a_{\ell}$.

Let us consider a fixed color configuration θ for the edges $a_1, a_2, \dots, a_{\ell}$. This fixed configuration, together with the fact that each cycle $\mu^{(i)}$ must have an *even* number of green edges, lead to the following number N_{θ} of possible configurations:

$$N_{\theta} = \prod_{i=1}^c 2^{k_i-1} = 2^{k-c} \tag{A.2}$$

as, once we choose the configurations of any $(k_i - 1)$ edges of a cycle $\mu^{(i)}$, the color of the remaining edge of this cycle is automatically determined by the mentioned restriction.

Since the constraint of having an even number of green edges in each cycle was already taken into account in eq. (A.2), there are 2^{ℓ} possible configurations θ 's for the edges $a_1, a_2, \dots, a_{\ell}$. Therefore the total number $f(\tilde{R})$ of graphs which do not contain any cycle with an odd number of green edges is given by

$$f(\tilde{R}) = 2^{\ell+k-c} = 2^{|E_{\tilde{R}}|-c(\tilde{R})} \tag{A.3}$$

where we have used relation (A.1a)

Notice that if we had considered a cycle basis which is not associated with some spanning tree of \tilde{R} , then it could eventually happen that one or more k_i 's vanish. But if $k_i = 0$ then all the edges of cycle i would belong to the set $\{a_1, a_2, \dots, a_\ell\}$. Consequently, we should replace the factor $2^{k_i-1} = 2^{-1}$ by just 1, and we should also substitute the $2^\ell \theta$'s configurations by $2^{\ell-1}$ (since, in this case, the edges a_i which belong to the cycle i must satisfy the restriction of having an even number of green edges). In this case N_θ would become $2^{k-(c-1)}$ and $f(\tilde{R}) = 2^{\ell-1} \times 2^{k-(c-1)} = 2^{\ell+k-c}$ would coincide with the result (A.3). If there were more cycles with null k_i 's, this reasoning would apply for each such cycle and we would recover, at the end, eq. (A.3).

We can, therefore, conclude that the result (A.3) is true for *any* cycle basis, or in other words, this formula depends only on the topology of the graph \tilde{R} , as it should be.

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