

Coniglio-Klein mapping in the metastable region

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We explicitly calculate the connectivity in the percolation problem defined by the Coniglio-Klein mapping of the Ising model on the Bethe lattice. We study the relation between thermal correlations and connectivity in the (T, H) region where the system is metastable, with the aim of interpreting the mean-field spinodal line with a percolation line of the same sort. We find that the extension of the mapping to the metastable region is characterized by a nontrivial feature, i.e., the simultaneous presence of two infinite percolating clusters of opposite spin. This feature destroys the usual equivalence between correlation and connectivity. A different relation between thermal and percolative quantities, which reduces to the known relation in the stable region, can be obtained if the cross correlation between the two infinite clusters is taken into account.

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I. INTRODUCTION

The geometric description of thermal quantities, initiated by Fortuin and Kasteleyn [1] and developed by Coniglio and Klein [2] and many others [3–6], has contributed to a deeper understanding of critical phenomena. Thermal variables, such as magnetization and correlation functions, have been shown to be equivalent to percolative quantities, such as the strength of the infinite network and the pair connectivity. With a suitable choice of the percolation model, the critical point has been exactly mapped onto a percolation point. Using such a mapping, the critical exponents have been shown to coincide with the percolation ones.

The mapping between thermal and percolative quantities allows one to identify (and visualize) the paths through which correlations propagate in the system. The suitably defined percolation clusters act as independent units, completely uncorrelated among each other. Instead, the cluster elements are infinitely strongly correlated. Under such mapping, the thermal correlation length is connected to the average cluster size. The divergence of the correlation length at the critical point is equivalent to the formation of a spanning cluster. According to the mapping, the critical point is the only percolation point in the region where the system is stable. Indeed, with the exclusion of the critical isochore, the system can be partitioned in a collection of finite clusters plus one infinite cluster, the latter accounting for the infinite-range correlation associated with the presence of a nonzero order parameter.

In the Ising model with coupling constant J , the equivalence between thermal and percolative quantities is achieved when nearest-neighbor parallel spins are connected by random bonds with probability $p_{ck} = 1 - e^{-2\beta J}$ [2], where $\beta = 1/k_B T$. In the presence of an external magnetic field H , visualized as an external spin (named ghost spin) $s_{gh} = H/|H|$ parallel to H , spins are connected with s_{gh} with probability $q_{ck} = 1 - e^{-2\beta|H|}$. Clusters are defined by con-

nected spins. Using this bond definition, the probability for each spin to belong to the infinite cluster exactly maps onto the magnetization and so does the probability of two spins to belong to the same cluster (the connectivity) with the thermal correlation.

Based on such a geometric description, a cluster dynamics for the thermal Ising model has been introduced by Swendsen and Wang [6] and recently optimized [7]. In this dynamics all spins belonging to the same cluster are flipped with probability 1/2, while spins in the infinite cluster never flip. Such artificial dynamics dramatically reduces the critical slowing down near the critical point for Monte Carlo simulations. More recently [8–11,7], the same formalism has been analytically extended to frustrated systems.

In mean-field models the correlation length diverges not only at the critical point, but also along the spinodal line, which delimits the region of metastability in the phase diagram. According to the previously discussed mapping, in the mean field one would expect to be able to associate the spinodal line with a percolation line. The equivalence between the thermal correlation length and connectivity in the metastable region is the main point of this article. Ray and Klein [12,13] showed that in order to maintain the spinodal line as a percolation line it is necessary to redefine the bond probability as $1 - e^{-2\beta J(1-M)}$, where M is the magnetization. In the present paper we consider the consequences of using the Coniglio-Klein mapping, i.e., we retain the definition of p_{ck} and q_{ck} . We study the Ising model on the Cayley tree to implement directly into the model the mean-field approach. We find that in extending the mapping to the metastable region, an additional nontrivial feature that destroys the equivalence between the correlation and connectivity shows up. The thermal correlation and connectivity are not equal anymore due to the anticorrelation that develops in the presence of two distinct infinite clusters. One is formed by spanning parallel spins and the other by isolated clusters of spins of opposite sign connected through the ghost site. This result is particularly interesting for its analogies to the similar structure of the correlation and connectivity that develops in spin glasses [14].

To explicitly calculate the connectivity in the metastable region we first derive (Sec. II) the expressions for the connectivity on the Cayley tree for a very general model of

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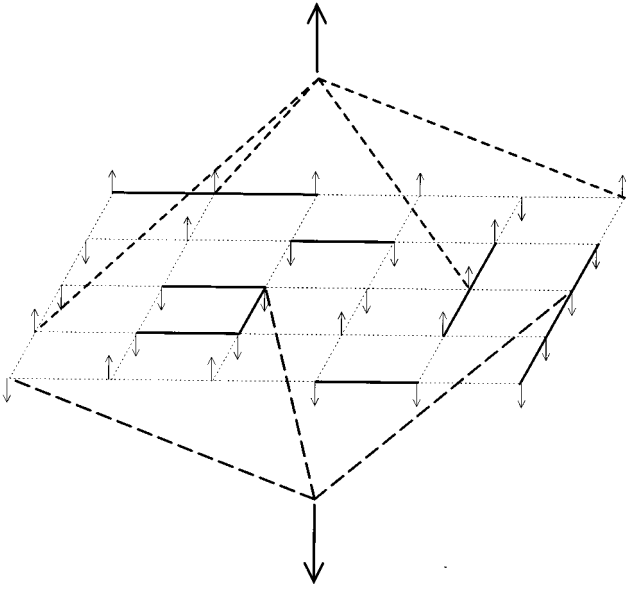


FIG. 1. Connectivity of a CSR model generally defined with two ghosts: Bonds are present within the lattice between NN parallel sites with probability π (full lines) and between sites \uparrow (\downarrow) and the \uparrow ghost (\downarrow ghost) with probability σ_{\uparrow} (σ_{\downarrow}) [dashed lines] [σ_1 (long-dashed lines)].

correlated-site-random-bond (CSR) percolation in the presence of two external ghosts. The extension of the known CSR model to the case where two external ghost sites are simultaneously present is required in the modeling the peculiar structure of the spin system in the metastable region, where two infinite clusters of opposite sign coexist [4]. The reader interested only in the mapping between thermal and percolation quantities in the stable and metastable regions can start from Sec. III, where the general expressions for the connectivity derived in Sec. II are specialized to the Coniglio-Klein (CK) mapping case and compared with the corresponding thermal quantities.

II. CONNECTIVITY IN THE CSR MODEL WITH TWO GHOSTS

The calculation of percolative quantities such as the percolation line, connectivity, mean cluster size, and critical exponents on a Cayley tree is largely available in the literature for the random-site-random-bond model [15,16], in the presence of a ghost [1,17–20], and in the correlated case without a ghost [19,21–27]. For a very complete review see [28]. Using Essam's formalism we calculate the order parameter and the connectivity of a generic CSR percolation model with two ghosts (see Fig. 1).

The CSR model with two ghosts may be generally defined on a lattice where the sites may be of two types, distributed according to an assigned probability distribution. Bonds are thrown between nearest-neighbor (NN) sites of the same type, with a random probability π . Two external sites, one for each site type, are also defined and bonds are thrown between lattice sites and the external site of the same type with random probability σ . Clusters are thus defined as connected spins. We will focus our interest on the connectivity

of the model, i.e., on the calculation of the probability C_n for two sites, $n-1$ sites apart, to belong to the same cluster.

We solve the model on the Cayley tree of coordination γ (i.e., γ branches originate from each site). Each site can be either \uparrow or \downarrow . The distribution of sites in the lattice is defined by the quantities $P(\uparrow)$ and $P(\uparrow\uparrow)$, from which one can calculate any conditional probability $P_n(\uparrow|\uparrow)$ using the recursive relations

$$P_n(\uparrow\uparrow) = P_{n-1}(\uparrow\uparrow)P_1(\uparrow\uparrow) + P_{n-1}(\downarrow\uparrow)P_1(\uparrow\downarrow) \quad (1)$$

and the completeness equations

$$P_n(\downarrow\uparrow) = 1 - P_n(\uparrow\uparrow),$$

$$P(\uparrow)P_n(\downarrow\uparrow) = P(\downarrow)P_n(\uparrow\downarrow). \quad (2)$$

Let π be the probability of two parallel NN sites to be connected and σ_{\uparrow} (σ_{\downarrow}) the probability of an up (down) site to be connected with the up (down) ghost. The probability P_{\uparrow}^{∞} for a single site, labeled 0, to belong to the infinite up cluster is

$$P_{\uparrow}^{\infty} = P(\uparrow)[1 - (1 - \sigma_{\uparrow})Q_{\uparrow}^{\gamma}], \quad (3)$$

$$1 - Q_{\uparrow} = P(\uparrow\uparrow)[1 - (1 - \sigma_{\uparrow})Q_{\uparrow}^{\gamma-1}]. \quad (4)$$

Q_{\uparrow} can be interpreted as the probability that one branch, generated from an up site, is not connected to the up ghost. An analogous expression can be obtained for P_{\downarrow}^{∞} . For every γ Eq. (4) has a unique solution that satisfies $Q_{\uparrow} \leq 1$.

We now calculate the generalized connectivity C_n , defined as the probability for two sites, separated by $n-1$ other lattice sites, to belong to the same cluster. The two sites can be connected either via a continuous path of bonds in the lattice [$F_n(\uparrow)$ or $F_n(\downarrow)$], or through the ghost [$G_n(\uparrow)$ or $G_n(\downarrow)$] [29]. Thus C_n is the sum of four contributions

$$C_n = F_n(\uparrow) + F_n(\downarrow) + G_n(\uparrow) + G_n(\downarrow). \quad (5)$$

The expressions for $F_n(\uparrow)$ and $F_n(\downarrow)$ are straightforward; we have

$$F_n(\uparrow) = P(\uparrow)[P(\uparrow\uparrow)p_{ck}]^n, \quad (6)$$

and analogously for $F_n(\downarrow)$.

The calculation of $G_n(\uparrow)$ and $G_n(\downarrow)$ requires more care. Let us start with $G_n(\uparrow)$ by considering the path connecting site 0 with site n . We define $P_{n,s,t}$ as the probability of the site configuration in which sites $0, \dots, s$ are up, site $s+1$ is down, site $t-1$ is down, and sites t, \dots, n are up (see Fig. 2) with $t > s$. $P_{n,s,t}$ is

$$P_{n,s,t} = P(\uparrow)P(\uparrow\uparrow)^{s+n-t}P(\downarrow\uparrow)P_{t-(s+2)}(\downarrow\downarrow)P(\uparrow\downarrow). \quad (7)$$

The probability of the configuration with exactly i up sites bound to the origin in the direction $0-n$ (and thus $i \leq s$) and exactly $n-j$ up sites bound to site n (so that $j \geq t$) is

$$P_{n,s,t,i,j} = P_{n,s,t} \pi^i (1 - \pi)^{\phi} (1 - \pi)^{\psi} \pi^{n-j}, \quad (8)$$



FIG. 2. In this configuration sites $0, \dots, s-1$ are \uparrow , sites s and $t-1$ are \downarrow ($t > s$), and sites t, \dots, n are \uparrow . Sites $0, \dots, i$ are bound by bonds within the lattice, as well as sites j, \dots, n . $\gamma-2$ branches (other than the NN present in the figure) originate from each site $1, \dots, n-1$, while $\gamma-1$ branches originate from sites 0 and n . The probability of this configuration (with no consideration of bonds with the ghost site) is $P_{n,s,t,i,j}$.

where $\phi = 1 - \delta_{i,s}$ and $\psi = 1 - \delta_{j,t}$ take into account the occurrence of $i=s$ and $j=t$ cases (we use the function $\delta_{l,m} = 1$ if $l=m$ and zero otherwise).

We now evaluate the probability of sites 0 and n to be connected to each other through the ghost in the configuration $P_{n,s,t,i,j}$. Site 0 is connected with the ghost in one of the following cases: (i) directly, (ii) through one of its i bounded NNs, or (iii) if at least one of the $(i+1)(\gamma-2)+1$ branches originating from sites $0, \dots, i$ goes to the ghost. If we define the quantity $q_{\uparrow} = (1 - \sigma_{\uparrow})Q_{\uparrow}^{\gamma-2}$, the probability of site 0 not to be connected with the ghost (i.e., none of the previous conditions occurring) is

$$(1 - \sigma_{\uparrow})^{i+1} Q_{\uparrow}^{(i+1)(\gamma-2)+1} = q_{\uparrow}^{i+1} Q_{\uparrow}. \quad (9)$$

If exactly i sites in the line $0, \dots, n$ are bound to site 0 and $n-j$ to site n , the probability of both 0 and n being connected to the ghost is

$$G_{n,s,t,i,j} = P_{n,s,t,i,j} (1 - q_{\uparrow}^{i+1} Q_{\uparrow}) (1 - q_{\uparrow}^{n-j+1} Q_{\uparrow}). \quad (10)$$

In order to obtain $G_n(\uparrow)$ we sum the previous expressions over all the possible values of the variables i, j, s, t . We also take into account the configuration in which all the sites in the line $0, \dots, n$ are up, but not all the bonds are present. We thus obtain

$$\begin{aligned} G_n(\uparrow) &= \sum_{s=0}^{n-2} \sum_{t=s+2}^n \sum_{i=0}^s \sum_{j=t}^n G_{n,s,t,i,j} \\ &+ P(\uparrow) P(\uparrow|\uparrow)^n \sum_{i=0}^{n-1} \sum_{j=i+1}^n \pi^i (1 - \pi)^{2 - \delta_{i+1,j}} \pi^{n-j}. \end{aligned} \quad (11)$$

The factor $(1 - \pi)^{2 - \delta_{i+1,j}}$ in the second term states that only one bond is absent when $i+1=j$.

The calculation of the two terms in Eq. (11) is derived in the Appendix. We report here only the final expression for $G_n(\uparrow)$:

$$\begin{aligned} G_n(\uparrow) &= A_1 P_n(\uparrow|\uparrow) + A_2 [P_1(\uparrow|\uparrow)]^n + A_3 [P_1(\uparrow|\uparrow)\pi]^n \\ &+ A_4 [P_1(\uparrow|\uparrow)\pi q_{\uparrow}]^n + A_5 [P_1(\uparrow|\uparrow)\pi q_{\uparrow}]^n n + A_6. \end{aligned} \quad (12)$$

The complete expressions of the coefficients A_1, \dots, A_6 , which are rational function of $P(\uparrow), P(\uparrow|\uparrow), Q_{\uparrow}, q_{\uparrow}, \pi$, are reported in the Appendix.

The calculation of $G_n(\downarrow)$ exactly parallels the one for $G_n(\uparrow)$. The final result for $G_n(\downarrow)$ is an expression similar to Eq. (12), with the exchange of the symbols \uparrow and \downarrow . We call B_1, \dots, B_6 the properly defined coefficients for $G_n(\downarrow)$.

Summing the two terms $G_n(\uparrow)$ and $G_n(\downarrow)$ with the two terms $F_n(\uparrow)$ and $F_n(\downarrow)$ [see Eq. (6)], we obtain the final result for the connectivity:

$$\begin{aligned} C_n &= A_1 P_n(\uparrow|\uparrow) + A_2 [P_1(\uparrow|\uparrow)]^n + [A_3 + P(\uparrow)] [P_1(\uparrow|\uparrow)\pi]^n \\ &+ A_4 [P_1(\uparrow|\uparrow)\pi q_{\uparrow}]^n + A_5 [P_1(\uparrow|\uparrow)\pi q_{\uparrow}]^n n + A_6 \\ &+ B_1 P_n(\downarrow|\downarrow) + B_2 [P_1(\downarrow|\downarrow)]^n + [B_3 + P(\downarrow)] \\ &\times [P_1(\downarrow|\downarrow)\pi]^n + B_4 [P_1(\downarrow|\downarrow)\pi q_{\downarrow}]^n \\ &+ B_5 [P_1(\downarrow|\downarrow)\pi q_{\downarrow}]^n n + B_6. \end{aligned} \quad (13)$$

III. CONIGLIO-KLEIN MAPPING IN THE STABLE AND METASTABLE REGIONS

The mean-field approximation for the Ising model, with the Hamiltonian $\mathcal{H} = J \sum_{NN} s_i s_j + H \sum_i s_i$, may be stated [30,31] through the Bethe-Peierls equations

$$P(+)=\frac{z(z y+1)}{z(z y+1)+z+y}, \quad (14)$$

$$P_1(+|+)=\frac{z y}{z y+1},$$

$$z=f(z)=\mu\left(\frac{z y+1}{z+y}\right)^{\gamma-1}, \quad (15)$$

where γ is the coordination number of the lattice, $y = e^{(2\beta J)}$, $\mu = e^{(2\beta H)}$, $P(+)$ is the probability of a single spin to be in the $s = +1$ state, and $P_1(+|+)$ is the conditional probability of a spin to be in the $s = +1$ state, knowing that one of its NNs is in the $s = +1$ state.

Equations (14) and (15) are exact on the γ Cayley tree since the mean-field approximation is equivalent to neglecting the correlation loops present in a generic lattice. As is known for the van der Waals and Curie-Weiss equations, Eq. (15) has one or three solutions, according to the values of the variables H and T . When three solutions are available they are respectively identified with stable, unstable, and metastable states of the system. The critical point is found by imposing the collapse of the three solutions, i.e., through the conditions $H=0$ and $f'(1)=1$. The spinodal line, i.e., the limit of existence of a metastable state, is defined by the identity of two of the three solutions of Eq. (15) or through the condition of diverging susceptibility.

The magnetization M and the spin-spin correlation $S_n \equiv \langle s_0 s_n \rangle$ can be generally written as

$$M \equiv \langle s_0 \rangle = P(+)-P(-), \quad (16)$$

$$S_n = 2P(+P_n(+|+)) + 2P(-P_n(-|-)) + 1. \quad (17)$$

The isomorphism between the thermal Ising model and the percolative CSRB model under the Coniglio-Klein mapping can be stated through the equivalences

$$\begin{aligned} \uparrow \rightarrow +, \quad \downarrow \rightarrow -, \quad \pi \rightarrow p_{ck} &\equiv 1 - e^{-2\beta J} = 1 - y^{-1}, \\ \sigma_{\uparrow} \rightarrow q_{ck} &\equiv 1 - e^{-2\beta|H|} = 1 - \mu^{-1}, \quad H > 0 \\ \sigma_{\downarrow} &= 0, \quad H > 0, \\ \sigma_{\uparrow} = 0, \quad H < 0 \quad \sigma_{\downarrow} \rightarrow q_{ck} &\equiv 1 - e^{-2\beta|H|} = 1 - \mu, \quad H < 0. \end{aligned} \quad (18)$$

Note that since in the thermal model only one ghost is present, σ_{\uparrow} or σ_{\downarrow} is always zero.

The equivalence between thermal and percolative properties in the stable region has been extensively discussed in the past [2,6,3,5]. We briefly discuss here these well-known results using the formalism of Sec. II.

When bonds are thrown between parallel NN pairs of spins $s_i s_j$ and $s_i s_{gh}$, with probabilities p_{ck} and q_{ck} , two types of clusters are formed: (i) finite clusters of + and - spins and (ii) an infinite cluster of + spins (for a positive H) connected to the ghost site. The infinite cluster is percolating within the lattice via p_{ck} bonds (i.e., independently of the presence of q_{ck} bonds) if the condition $P(+|+)p_{ck}(\gamma - 1) > 1$ is satisfied.

Under the mapping M coincides with P_+^{∞} , as can be verified by substituting in Eqs. (3) and (4) the thermal expression for $\sigma, P(\uparrow), P(\uparrow|\uparrow)$, and π . Since $M = P_+^{\infty}$, the contribution of + and - finite-size clusters to the magnetization is zero because their size distributions are identical [4,5]. Under the CK mapping, thermal correlations, as measured by S_n , coincide with the connectivity, as measured by C_n . Indeed, the connectivity expression (13) coincides with the thermal correlation expression (17) once the values of the coefficients in Eq. (13) are evaluated under the CK mapping [Eqs. (18)],

$$\begin{aligned} A_1 &= 2P(\uparrow), \\ B_1 &= 2P(\downarrow), \\ A_3 &= -P(\uparrow), \\ B_3 &= -P(\downarrow), \\ A_6 + B_6 &= 1, \end{aligned} \quad (19)$$

$$A_2 = A_4 = A_5 = B_2 = B_4 = B_5 = 0,$$

and substituted into Eq. (13).

We now discuss the CK mapping in the metastable region ($H < 0, M > 0$). It has already been argued [4] that in the metastable region two infinite clusters of + and - spins are present: one infinite cluster of - spins connected to the ghost and one infinite cluster of + spins connected via p_{ck} bonds through the lattice. Here we show that the presence of two infinite clusters produces an additional effect that destroys the equivalence between the connectivity and thermal correlation and forces one to take into account the anticorrelation between the two infinite clusters.

The breakdown of the equivalence between S_n and C_n in the metastable region appears already in the relation connecting M and the strength of the infinite cluster. Indeed, as can be derived under the mapping (18), in the metastable region

$$M = P_+^{\infty} - P_-^{\infty}, \quad (20)$$

where P_{\pm}^{∞} is the probability that the spin is in a infinite \pm cluster.

In the limit of $n \rightarrow \infty$, $S_n = M^2 = P_+^{\infty 2} + P_-^{\infty 2} - 2P_+^{\infty}P_-^{\infty}$ [where we have used Eq. (20)]. Because only infinite clusters can give contributions to the connectivity for $n \rightarrow \infty$, we expect to find, together with the connectivity of the cluster of spin + (the $P_+^{\infty 2}$ term) and the cluster of - spins (the $P_-^{\infty 2}$ term), an additional *anticorrelation* resulting from the different signs of the spins between the two infinite clusters (the $-2P_+^{\infty}P_-^{\infty}$ term).

By using the mapping in Eq. (18) we now show that the correct relation between S_n and C_n is

$$S_n = C_n - 2G_n(\pm), \quad (21)$$

where $G_n(\pm)$ is the probability of two spins, $n-1$ sites apart, to belong to different infinite clusters. Using the formalism of Sec. II and the results derived in the Appendix, $G_n(\pm)$ can be explicitly calculated. This computation leads, once the mapping is considered, to the expression

$$\begin{aligned} G_n(\pm) &= \tilde{C}_1 P_n(+|+) + \tilde{C}_2 [P(+|+)]^n + \tilde{C}_3 [P(-|-)]^n \\ &\quad + \tilde{C}_4 [P(+|+)p_{ck}q_+]^n + \tilde{C}_5 [P(+|+)p_{ck}q_+]^n n \\ &\quad + \tilde{C}_6, \end{aligned} \quad (22)$$

with $\tilde{C}_1, \dots, \tilde{C}_6$ properly defined in the following equations in the metastable region under the CK mapping [Eqs. (18)]:

$$\tilde{A}_1 + P(+)/P(-)\tilde{B}_1 + \tilde{C}_1 = 4P(+), \quad (23)$$

$$\tilde{A}_2 + \tilde{C}_2 = 0,$$

$$\tilde{B}_2 + \tilde{C}_3 = 0,$$

$$\tilde{A}_3 + P(+)=0, \quad (23)$$

$$\tilde{B}_3 + P(-)=0,$$

$$\tilde{A}_4 + \tilde{B}_4 + \tilde{C}_4 = 0,$$

$$\tilde{A}_5 + \tilde{B}_5 + \tilde{C}_5 = 0,$$

$$\tilde{A}_6 + \tilde{B}_6 + \tilde{C}_6 + \tilde{B}_1[1 - P(+)/P(-)] = 3 - 4P(+).$$

$\tilde{A}_1, \dots, \tilde{B}_1, \dots$ are the values of the coefficients of Eq. (13) obtained by substituting the mapping in the metastable region. By substituting Eq. (22) into Eq. (21) and using the relations of Eq. (23), we recover Eq. (17) [32].

Equation (21), the main result of this paper, implies that the spinodal line, along which the susceptibility diverges, is not a percolation line due to the presence of the $-2G_n(\pm)$ term. The thermal correlation in the metastable region can be

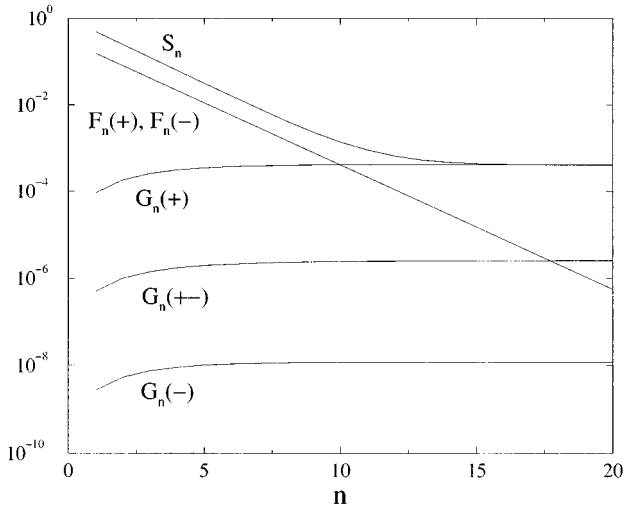


FIG. 3. Thermal correlation length S_n in the metastable region ($M > 0, H < 0$). S_n is the sum of finite connectivity [$F_n(+), F_n(-)$], infinite cluster connectivity [$G_n(+)$], and connectivity through the ghost [$G_n(-)$], minus the anticorrelation term [$G_n(\pm)$].

seen as propagating via the finite clusters (of both plus and minus spins) and via the two infinite clusters of opposite sign. At the same time, an anticorrelation develops between spins belonging to the two infinite clusters, destroying the equivalence between S_n and C_n . An example of all the connectivity contributions to the correlation function close to the spinodal line is shown in Fig. 3.

IV. CONCLUSIONS

In this article we have discussed the extension of the mapping between thermal and percolative quantities to the metastable region in an Ising model, trying to interpret the spinodal line in terms of geometrical quantities. Indeed, in mean-field models, where the concept of spinodal line is well defined, the scattered intensity diverges not only at the critical point but also along the spinodal line, the limit of thermodynamic stability. The divergence of the scattered intensity signals the development of an infinite-range correlation in the system, which in the percolative approach is usually interpreted in terms of the formation of a percolating cluster. In this paper we have shown that this is not the case and that the divergence in the connectivity length is more subtle, being associated with the development of a cross correlation between two infinite clusters of opposite sign.

By solving the percolation problem defined by the CK mapping on the Bethe lattice, we have explicitly calculated the contributions to the connectivity arising from finite clusters and from the two infinite clusters of opposite spin. Indeed, in the metastable region of the phase diagram, two different infinite clusters coexist [4]. Both infinite clusters are well beyond the percolation threshold at the spinodal. Thus only the critical point can be associated with a percolation point in the CK approach. We have shown that the equivalence between the thermal correlation and connectivity is lost in the metastable region due to the presence of the two coexisting infinite clusters. As shown in Eq. (21), a dif-

ferent relation between thermal and percolative quantities, which reduces to the known relation in the stable region, can be obtained if the cross correlation between the two infinite cluster is taken into account.

From a heuristic point of view, finite clusters can be thought of as independent units of infinitely strongly correlated spins of the same sign that may stay in either of the two states (+ and -) with equal probability. The contribution to the magnetization arising from finite clusters averages to zero. Instead, infinite clusters are responsible for the finite magnetization of the sample and remain always in the same spin state. An analogous qualitative argument can be put forth for the spin-spin correlation S_{ij} . Spins belonging to different clusters do not contribute to S_{ij} because they contribute with plus one [(+,+) (-,-)] or with minus one [(+, -) (-,+)] with equal probability. This argument holds in the stable region even when one of the two clusters is the infinite cluster, in which case the two possible states are again equiprobable. In the metastable region, the case of two never flipping infinite clusters arises. The correlation between spins belonging to these two infinite clusters of opposite spin never averages out since S_{ij} is always equal to -1. This (negative) contribution to the thermal correlation has to be added to the single cluster connectivity, as expressed by the $-G_{\pm}$ term in Eq. (21).

The relation between the connectivity and correlation in the metastable region, is similar to the situation encountered in the percolative study of frustrated systems, such as spin glasses. In that case, the strongly correlated clusters are composed of spins of opposite sign. The presence of spins of both sign in the same cluster introduces, like in the case of two infinite clusters in the metastable region, an anticorrelation within the same cluster. This anticorrelation breaks down, even in the spin-glass case, the equivalence between the correlation and connectivity. Indeed, Eq. (21) matches the more general context of the Ising spin-glass model [14] where the correlation function is given by

$$S_n = P_n^{\parallel} - P_n^{\#}, \quad (24)$$

where P_n^{\parallel} ($P_n^{\#}$) is the probability that spins $n-1$ sites apart are parallel (antiparallel) and belong to the same cluster. Considering the two infinite clusters present in the metastable region as one infinite cluster of up and down spins, Eq. (21) coincides with Eq. (24).

A similar situation may characterize the application of the CK mapping to off-lattice systems for realistic interparticle potentials. The presence of a hard-core region around each particle may again be visualized as a persistent anticorrelation to be taken into account properly.

APPENDIX

This appendix is aimed at deriving Eq. (12) for $G_n(\uparrow)$ from Eq. (11). The two terms in Eq. (11) reduce either to the geometrical sum or to sums solvable by recursion. We first calculate the first term on the right-hand side (rhs) of Eq. (11), starting by sums with indices i, j , namely [using Eqs. (10) and (8)],

$$\begin{aligned} \sum_{i=0}^s \sum_{j=t}^n G_{n,s,t,i,j} &= P_{n,s,t} \sum_{i=0}^s \pi^i (1-\pi)^\phi \\ &\times (1 - Q_\uparrow q_\uparrow q_\uparrow^i) \sum_{j=t}^n \pi^{n-j} (1-\pi)^\psi \\ &\times (1 - Q_\uparrow q_\uparrow q_\uparrow^{n-j}). \end{aligned} \quad (\text{A1})$$

The factor ϕ of Eq. (A1) is computed by dividing the sum in $0 \leq i \leq s$ into the two parts $0 \leq i \leq s-1$ (which is a geometrical sum) plus the single term $i=s$, and analogously for the factor ψ , which is computed by dividing the sum in $t \leq j \leq n$ into the sum $t+1 \leq j \leq n$ plus the single term $j=t$. The same argument works for the sums in the second term of rhs of Eq. (11). After executing all sums in i and j of Eq. (11) we obtain

$$\begin{aligned} G_n(\uparrow) &= a_0 \sum_{s=0}^{n-2} \sum_{t=s+2}^n P_{n,s,t} [a_1 + (\pi q_\uparrow)^s] [a_2 + (\pi q_\uparrow)^{n-t}] \\ &+ P(\uparrow|\uparrow)^n [b_1 + b_2 \pi^n + b_3 (q_\uparrow \pi)^n + b_4 n (q_\uparrow \pi)^n]. \end{aligned} \quad (\text{A2})$$

The $a_0, a_1, a_2, b_1, \dots, b_4$ are suitable coefficients, expressed only via $P(\uparrow), P(\uparrow|\uparrow), Q_\uparrow, q_\uparrow, \pi$ (see below). We now substitute Eq. (7) into Eq. (A2) and define the new variables $t' = t - (s+2)$ and $n' = n - (s+1)$. We can write the first term on rhs of Eq. (A2) as

$$a'_0 P(\uparrow|\uparrow)^n \sum_{n'=0}^{n-1} [a_1 + (\pi q_\uparrow)^{n-n'-1}] [a_2 \mathcal{R}_1 + (\pi q_\uparrow)^{n'} \mathcal{R}_2] \quad (\text{A3})$$

with a new coefficient a'_0 (see below) and with the definitions

$$\mathcal{R}_1 = \sum_{t'=0}^{n'-1} \frac{P_{t'}(\downarrow|\downarrow)}{P(\uparrow|\uparrow)^{t'}}, \quad (\text{A4})$$

$$\mathcal{R}_2 = \sum_{t'=0}^{n'-1} \frac{P_{t'}(\downarrow|\downarrow)}{[P(\uparrow|\uparrow)\pi q_\uparrow]^{t'}}. \quad (\text{A5})$$

The sums \mathcal{R}_1 and \mathcal{R}_2 may be calculated by recursion using Eq. (1). The result is

$$\mathcal{R}_1 = \frac{j_1 + j_2 P_{n'}(\downarrow|\downarrow)}{P(\uparrow|\uparrow)^{n'}}, \quad (\text{A6})$$

$$\mathcal{R}_2 = k_0 + \frac{k_1 + k_2 P_{n'}(\downarrow|\downarrow)}{[P(\uparrow|\uparrow)\pi q_\uparrow]^{n'}}, \quad (\text{A7})$$

with j_0, \dots, k_0, \dots defined below. The remaining sum over n' in Eq. (A3) can be evaluated in a very similar way. Substituting Eqs. (A6) and (A7) into Eq. (A3), this reduces to

$$P(\uparrow|\uparrow)^n \sum_{n'=1}^n \left(l_1 (\pi q_\uparrow)^{n'} + l_2 \frac{1}{P(\uparrow|\uparrow)^{n'}} + l_3 \frac{P_{n'}(\downarrow|\downarrow)}{P(\uparrow|\uparrow)^{n'}} \right.$$

$$\begin{aligned} &+ l_5 (\pi q_\uparrow)^n + l_6 \frac{1}{[P(\uparrow|\uparrow)\pi q_\uparrow]^{n'}} (\pi q_\uparrow)^n \\ &+ l_7 \frac{P_{n'}(\downarrow|\downarrow)}{[P(\uparrow|\uparrow)\pi q_\uparrow]^{n'}} (\pi q_\uparrow)^n \Big), \end{aligned} \quad (\text{A8})$$

with l_0, \dots defined below. Three of the terms in Eq. (A8) can be calculated as geometrical sums: One is trivial and the other two (with coefficients l_3 and l_7) exactly reduce to \mathcal{R}_1 and \mathcal{R}_2 , respectively [see Eqs. (A4) and (A5)]. The first term on the rhs of Eq. (A2) is thus completely calculated

$$\begin{aligned} &h_1 P_n(\uparrow|\uparrow) + h_2 P(\uparrow|\uparrow)^n + h_3 [P(\uparrow|\uparrow)\pi q_\uparrow]^n \\ &+ h_4 [P(\uparrow|\uparrow)\pi q_\uparrow]^n n + h_5. \end{aligned} \quad (\text{A9})$$

In order to obtain the final expression (12) for $G_n(\uparrow)$ we only have to add the second term on rhs of Eq. (A2).

We now list the coefficients previously defined in Secs. II and III and in this Appendix: coefficients defined by evaluating the sums in the variables i and j of Eqs. (11)–(A2),

$$x_1 = (1-\pi)Q_\uparrow / (1-\pi q_\uparrow), \quad (\text{A10})$$

$$x_2 = Q_\uparrow(1-q_\uparrow) / [q_\uparrow(1-\pi q_\uparrow)],$$

$$a_0 = \pi q_\uparrow (q_\uparrow x_2)^2,$$

$$a_1 = (q_\uparrow x_1 - 1) / q_\uparrow x_2, \quad (\text{A11})$$

$$a_2 = (q_\uparrow x_1 - 1) / q_\uparrow^2 \pi x_2,$$

$$b_1 = P(+)(1-q_\uparrow x_1) [1 - (1-\pi)q_\uparrow Q_\uparrow / (1-\pi q_\uparrow)],$$

$$b_2 = -P(\uparrow) [(1-q_\uparrow x_1) + (1-\pi)q_\uparrow^2 x_2 / (1-q_\uparrow)], \quad (\text{A12})$$

$$\begin{aligned} b_3 &= -P(\uparrow) [(1-\pi)(-q_\uparrow Q_\uparrow + q_\uparrow^2 Q_\uparrow x_1) / (1-\pi q_\uparrow) \\ &- (1-\pi)q_\uparrow^2 x_2 / (1-q_\uparrow)], \end{aligned}$$

$$b_4 = P(\uparrow)(1-\pi)q_\uparrow^2 Q_\uparrow x_2,$$

and coefficients defined by evaluating the sums in the variables s and t of Eqs. (11)–(12),

$$a'_0 = a_0 P(\uparrow) \frac{P(\downarrow|\downarrow)P(\uparrow|\downarrow)}{P(\uparrow|\uparrow)}, \quad (\text{A13})$$

$$\mathcal{F} = [P(\downarrow|\downarrow) - P(\downarrow|\uparrow)] / P(\uparrow|\uparrow), \quad (\text{A14})$$

$$\mathcal{G} = [P(\downarrow|\downarrow) - P(\uparrow|\downarrow)] / P(\uparrow|\uparrow)\pi q_\uparrow,$$

$$j_1 = 1/(1-\mathcal{F}), \quad (\text{A15})$$

$$j_2 = -1/(1-\mathcal{F}),$$

$$k_0 = \frac{1}{1-\mathcal{G}} \left(1 - \frac{P(\downarrow|\uparrow)}{1-P(\uparrow|\uparrow)\pi q_\uparrow} \right),$$

$$k_1 = \frac{1}{1-\mathcal{G}} \frac{P(\downarrow|\uparrow)}{1-P(\uparrow|\uparrow)\pi q_\uparrow}, \quad (\text{A16})$$

$$\begin{aligned}
k_2 &= \frac{-1}{1-\mathcal{G}}, \\
l_1 &= a'_0 a_1 k_0, \\
l_2 &= a'_0 a_1 (a_2 j_1 + k_1), \\
l_3 &= a'_0 a_1 (a_2 j_2 + k_2), \\
l_5 &= a'_0 k_0 \pi q_\uparrow, \\
l_6 &= a'_0 (a_2 j_1 + k_1) \pi q_\uparrow, \\
l_7 &= a'_0 (a_2 j_2 + k_2) \pi q_\uparrow, \\
h_1 &= (l_3 j_2 + l_7 k_2) P(\uparrow) / P(\downarrow), \\
h_2 &= \frac{l_1}{1-\pi q_\uparrow} - \frac{l_2 P(\uparrow|\uparrow)}{1-P(\uparrow|\uparrow)}, \\
h_3 &= \frac{l_1}{1-\pi q_\uparrow} - \frac{l_6 P(\uparrow|\uparrow) \pi q_\downarrow}{1-P(\uparrow|\uparrow) \pi q_\downarrow} + l_7 k_0,
\end{aligned} \tag{A17}$$

$$\begin{aligned}
h_4 &= l_5, \\
h_5 &= \frac{l_2 P(\uparrow|\uparrow)}{1-P(\uparrow|\uparrow)} + l_3 j_1 + \frac{l_6 P(\uparrow|\uparrow) \pi q_\downarrow}{1-P(\uparrow|\uparrow) \pi q_\downarrow} + l_7 k_1 \\
&\quad + (l_3 j_2 + l_7 k_2) \frac{P(\downarrow) - P(\uparrow)}{P(\downarrow)}, \\
A_1 &= h_1, \\
A_2 &= b_1 + h_2, \\
A_3 &= b_2, \\
A_4 &= b_3 + h_3, \\
A_5 &= h_4, \\
A_6 &= b_4 + h_5.
\end{aligned} \tag{A19}$$

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- [1] C. M. Fortuin and P. W. Kastaleyn, *Physica (Utrecht)* **57**, 536 (1972).
- [2] A. Coniglio and W. Klein, *J. Phys. A* **13**, 2775 (1980).
- [3] C.-K. Hu, *Phys. Rev. B* **29**, 5103 (1984).
- [4] A. Coniglio, F. de Liberto, G. Monroy, and F. Peruggi, *J. Phys. A* **22**, L837 (1989).
- [5] J.-S. Wang, *Physica A* **161**, 249 (1989).
- [6] R. H. Swendsen and J.-S. Wang, *Phys. Rev. Lett.* **58**, 86 (1987).
- [7] T. B. Liverpool and S. C. Glotzer, *Phys. Rev. E* **53**, R4255 (1996).
- [8] A. Coniglio, *Nuovo Cimento D* **16**, 1027 (1994).
- [9] V. Cataudella, G. Franzese, M. Nicodemi, A. Scala, and A. Coniglio, *Phys. Rev. Lett.* **72**, 1541 (1994).
- [10] V. Cataudella, G. Franzese, M. Nicodemi, A. Scala, and A. Coniglio, *Nuovo Cimento* **16**, 1259 (1994).
- [11] V. Cataudella, G. Franzese, M. Nicodemi, A. Scala, and A. Coniglio, *Phys. Rev. E* **54**, 175 (1996).
- [12] W. Klein, *Phys. Rev. Lett.* **65**, 1462 (1990).
- [13] T. S. Ray and W. Klein, *J. Stat. Phys.* **61**, 891 (1990).
- [14] S. C. Glotzer and A. Coniglio, *Comput. Mater. Sci.* **4**, 325 (1995).
- [15] M. E. Fisher and J. W. Essam, *J. Math. Phys.* **2**, 609 (1961).
- [16] D. Stauffer, *Introduction to Percolation Theory* (Taylor & Francis, London, 1985).
- [17] M. R. Giri, M. J. Stephen, and G. S. Grest, *Phys. Rev. B* **16**, 4971 (1977).
- [18] R. B. Griffiths, *J. Math. Phys.* **8**, 484 (1967).
- [19] H. Kunz and B. Souillard, *J. Stat. Phys.* **19**, 77 (1978).
- [20] P. J. Reynolds, H. E. Stanley, and W. Klein, *J. Phys. A* **10**, L203 (1977).
- [21] A. Coniglio, *J. Phys. A* **8**, 1773 (1975).
- [22] A. Coniglio, *Phys. Rev. B* **13**, 2194 (1976).
- [23] A. Coniglio, *Commun. Math. Phys.* **51**, 315 (1976).
- [24] A. Coniglio, *Ann. Isr. Phys. Soc.* **2**, 874 (1978).
- [25] A. Coniglio, C. R. Nappi, F. Peruggi, and L. Russo, *J. Phys. A* **10**, 205 (1977).
- [26] A. Coniglio and J. W. Essam, *J. Phys. A* **10**, 1917 (1977).
- [27] J. L. Lebowitz and O. Penrose, *J. Stat. Phys.* **16**, 321 (1977).
- [28] J. W. Essam, *Rep. Prog. Phys.* **43**, 833 (1980).
- [29] G_n describes the connectivity via the ghost. If the two sites are connected both via a continuous path on the lattice and through the ghost, we consider such connectivity in F_n .
- [30] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).
- [31] C. Domb, *Adv. Phys.* **9**, 245 (1960).
- [32] In showing the identity (21) it is useful to make use of the relations $P(+|+)q_+ = P(-|-)q_-$ and $P_n(-|-) = P(+|+)P(-)P_n(+|+) + 1 - P(+|+)P(-)$.