Cluster Percolation and
Thermal Critical Behaviour

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Abstract:

Continuous phase transitions in spin systems can be formulated as percolation of suitably defined clusters. We review this equivalence and then discuss how in a similar way, the color deconfinement transition in SU(2) gauge theory can be treated as a percolation phenomenon. In the presence of an external field, spin systems cease to show thermal critical behavior, but the geometric percolation transition persists (Kertész line). For $H \neq 0$, we study the relation between percolation and pseudocritical behavior, both for continuous and first order transitions, and show that it leads to the necessity of an $H$-dependent cluster definition. A viable formulation of this kind could serve as definition of deconfinement in QCD with dynamical quarks.

1. Introduction

Critical phenomena in spin systems and elsewhere are usually described in terms of spontaneous symmetry breaking or of singular behavior of the partition function. On the other hand, the size of domains of parallel spins generally increases near criticality, and so the search for a geometric “connectivity” formulation has been a long standing challenge. For some classes of systems, the problem is solved, and I begin by recalling how this is done.

The Ising model is defined by the Hamiltonian

$$\mathcal{H}(T, H) = -J \sum_{<ij>} s_i s_j - H \sum_i s_i; \quad s_i = \pm 1$$

which is used to calculate the partition function

$$Z(T, H) = \sum_{\{s_i\}} \exp\{-\beta \mathcal{H}(T, H)\}; \quad \beta \equiv 1/T;$$

here $J$ denotes the nearest neighbor spin-spin coupling and $H$ an external field. Given $Z(T, H)$, the magnetization and (isothermal) susceptibility are obtained as

$$m(T, H) = (\partial \log Z/\partial H)_T, \quad \chi(T, H) = (\partial m/\partial H)_T.$$
For vanishing external field, $H = 0$, the Ising model leads to a critical point $T = T_c$: for $T < T_c$, the $Z_2$ symmetry of the Hamiltonian $\mathcal{H}(T, 0)$ is spontaneously broken by the state of the system. The magnetization becomes the order parameter for the transition and vanishes for $T \to T_c$, while the susceptibility diverges there:

$$m(T, 0) \sim (T_c - T)\beta, \quad T \leq T_c; \quad \chi(T, 0) \sim |T_c - T|^\gamma.$$  \hfill (4)

The critical exponents $\beta$ and $\gamma$ specify the critical behavior and define the universality class of the transition.

It was shown by Fortuin and Kasteleyn [1] that the partition function of the model, given in Eq. (2) as sum over spin configurations, can for $H = 0$ be equivalently written as a sum over configurations of clusters containing $n$ lattice points. In the resulting form

$$Z(T, 0) = \sum_n \{ \prod_{<ij>} p_b \prod_{<ij>} (1 - p_b)^2 c(n) \}, \hfill (5)$$

$p_b \equiv 1 - \exp\{-2\beta J\}$ defines a bond weight between adjacent sites, while $n_{ij} = 1(0)$ specifies whether two sites are bonded or not. The number of $n$-clusters is given by $c(n)$.

In percolation theory, the observable corresponding to the order parameter is the percolation strength $P(T)$, defined as the probability that a given site belongs to a percolating cluster. In place of the susceptibility we now have the average cluster size $S(T)$; in the percolation region only finite clusters are included in the averaging. Using the FK formalism, Coniglio and Klein [2] showed that the percolation point coincides with the thermal critical temperature $T_c$, and that the percolation behavior is governed there by

$$P(T) \sim (T_c - T)\beta, \quad T \leq T_c; \quad S(T) \sim |T_c - T|^\gamma,$$  \hfill (6)

where $\beta$ and $\gamma$ are the usual thermal Ising exponents. For the Ising model, thermal critical behavior can thus be equivalently described as percolation of FK clusters.

A non-vanishing external field, $H \neq 0$, explicitly breaks the previous $Z_2$ symmetry of the Hamiltonian, and as a result, partition function and thermodynamic observables become analytic: there is no more thermal critical behavior. The magnetization now never vanishes; $H$ aligns some spins at any temperature (see Fig. 1).

However, the percolation transition persists also for $H \neq 0$. For any value of $H$ there exists a percolation point $T_p(H)$, such that for $T \leq T_p$ there is percolation and for $T > T_p$ not [3]. The critical behavior along the “Kertész line” $T_p(H)$ (see Fig. 1) is now determined by percolation critical exponents, so that the transition is no longer in the Ising universality class.

We note here that the equivalence between thermal and percolation behavior can in fact be restored if clusters are not required to be spatially connected. The introduction of an $H$-dependent ghost spin not on the lattice but able to couple to any lattice site allows spatially disjoint sites to form a cluster [4] and thus leads to percolation for all $H \neq 0$. We are here interested in the relation between spatial connectivity and thermal behavior; therefore we shall not pursue the ghost spin approach any further.

One major reason for our study is to address critical behavior in finite temperature QCD; let us therefore elaborate a little the problems which arise there. The constituents of strongly interacting matter, the hadrons, are finite size color-neutral bound states of
two (mesons) or three (nucleons) colored quarks coupled by colored gluons. At high density, when the hadrons strongly overlap, each quark finds in its immediate vicinity many others, so that a partitioning into subsets of two or three quarks in a given volume no longer makes any sense, suggesting that we now have quark matter. High temperatures lead through particle-antiparticle production to high density. Hence we expect at sufficiently high temperatures a transition from hadronic matter, with color-neutral hadrons as constituents, to a plasma of unbound colored quarks and gluons. One of the basic issues of strong interaction thermodynamics is this quark-hadron transition.

The theory of strong interactions, quantum chromodynamics (QCD), is defined by the QCD Lagrangian $\mathcal{L}(m_q)$, which contains the bare quark mass as an open parameter. In QCD thermodynamics, two limits are of particular interest. For massless quarks, $m_q = 0$, $\mathcal{L}(0)$ is invariant under chiral transformations. This chiral symmetry is spontaneously broken for $T < T_\chi$: through a surrounding gluon cloud, the quarks acquire a dynamically generated ‘constituent quark’ mass $M_q$, which essentially determines the mass of the conventional hadrons. Thus the mass of a nucleon as three quark bound state is approximately $3M_q$. At $T = T_\chi$, chiral symmetry is restored, $M_q \to 0$ and hadrons dissolve into quarks and gluons. In the opposite limit, for $m_q \to \infty$, the quarks drop out and QCD becomes a (non-Abelian) SU(3) gauge theory, which describes a system of interacting gluons. At low temperatures, these bind to form ‘glueballs’ as the hadrons of the theory. The resulting Lagrangian has a global $Z_3$ symmetry. For some $T \geq T_c$, this symmetry is spontaneously broken; color screening causes the colorless glueballs to dissolve into colored gluons, corresponding to the onset of color deconfinement. QCD thus leads to two genuine phase transitions:

- for $m_q = 0$, chiral symmetry restoration at $T_\chi$, corresponding to the vanishing of the constituent quark mass;
- for $m_q = \infty$, spontaneous $Z_3$ breaking at $T_c$ corresponding to the onset of color deconfinement in pure gauge theory.

In the real world, $m_q$ is small but finite; what happens then? For three massless quark flavors, the $Z_3$ transition is first order, so a discontinuity will persist for some range of masses $m_q^{\text{end}} < m_q$. For $m_q < m_q^{\text{end}}$, there is no further thermal critical behavior, which means that there is no true phase transition separating hadronic matter and quark-gluon
plasma (see Fig. 2). Is the transition from one state to the other then just a rapid cross-over? We would like to speculate that it is the Kertész line of QCD, corresponding to the onset of percolation for clusters of deconfined matter, and we have carried out some preliminary studies to address this idea.

2. Percolation and Deconfinement

As a simplified model, we consider here pure SU(2) gauge theory, which describes a system of interacting gluons of three different colors. Given such a medium at temperature $T$, we denote by $V(r, T)$ the potential between two static color charges $Q$ and $\bar{Q}$ separated by a distance $r$. Below a certain critical temperature $T_c$, there is confinement: the potential rises linearly with distance, so that $V(r, T) \to \infty$ for $r \to \infty$. Above $T_c$, color screening limits the range of the potential, so that now $V(r, T) \to g(T)$ for $r \to \infty$, with a finite $g(T) > 0$. The Polyakov loop expectation value, defined by

$$L(T) = \lim_{r \to \infty} \exp\{-V(r, T)/T\},$$

thus vanishes for $T \leq T_c$, i.e., in the confinement region, and takes on a non-zero value for $T > T_c$, when deconfinement set in. Hence it is the deconfinement order parameter.

In the lattice formulation of finite temperature QCD, one studies systems in the usual three space dimensions, with one additional dimension specifying the temperature. A Polyakov loop becomes in lattice SU(2) an up or down spin of arbitrary amplitude, associated to a given spatial lattice site and oriented in the temperature direction; the expectation value $L(T)$ is the average over all spatial lattice sites. Polyakov loop configurations on a given spatial lattice thus form something like a continuous spin Ising model, and it was therefore conjectured that the deconfinement transition in SU(2) gauge theory is in the universality class of the Ising model. This conjecture was subsequently confirmed by extensive lattice studies, showing that the critical exponents of the two models agree with remarkable precision.

We now would like to check if the deconfinement transition can also be described as percolation of like-sign Polyakov loop clusters. The first question to be addressed is the generalization of the global FK bond weight $1 - \exp\{-2J/T\}$ of the conventional Ising model with $s_i = \pm 1$ to the case where the amplitude of the spin becomes a local variable.
It was shown in both analytic and numerical studies of the continuous spin Ising model \[10\] that percolation and the thermal transition in fact become equivalent if the bond weights are taken to have the local form 
\[
1 - \exp\{-(2J/T)s_is_j\}
\]
for adjacent like-sign spins.

Turning to SU(2) gauge theory, we therefore start with the local FK bond weight 
\[p(i, j) = 1 - \exp\{2\kappa L_i L_j\}\]
expressed in terms of the local values \(L_i, L_j\) of like-sign Polyakov loops on adjacent spatial lattice sites \(i, j\); the variable \(\kappa\) must take into account the temperature dependent Polyakov loop coupling. The generalization to SU(2) thus leads to two basic problems: how can one determine the functional form of \(\kappa(T)\), and is it justified to approximate the correlations provided by the theory to only nearest neighbor interactions? In the strong coupling limit \[11\], one finds for \(N_T = 2\) that \(\kappa(T) \simeq (\beta(T)/2)^2\), where \(\beta(T)\) is the known temperature dependent coupling in the SU(2) gauge theory action. Using this relation, we thus generate SU(2) configurations at different temperatures and study the clustering properties. The results \[8\] show overall agreement, but some discrepancies in details; in particular, the critical couplings for the thermal transition and for deconfinement are obtained with very high precision and disagree slightly.

It therefore seems worthwhile to consider a formulation in which the strong coupling approximation and the restriction to nearest neighbor interactions are removed. This can be done in an effective spin description, in which the thermal system is parametrized in a spin model allowing longer range interactions as well, with up to 20 different couplings between different spins \[9\]. The values of these couplings are then determined numerically near the thermal critical point which in turn provides generalized bond weights \(\kappa_n\),

\[p(i, i + 1) = 1 - \exp\{-2\kappa_1 L_i L_{i+1}\},\]
\[p(i, i + 2) = 1 - \exp\{-2\kappa_1 L_i L_{i+2}\}, \ldots\] \(8\)

The resulting agreement between the critical thermal and percolation parameters is excellent, as seen in Table 1. The approach used here does not solve the question of how to define in general the FK bond weights in terms of the SU(2) Lagrangian; but it does show that the equivalence between thermal and geometric descriptions can be established numerically.

| Critical point          | \(\beta/\nu\)     | \(\gamma/\nu\)   | \(\nu\)     |
|------------------------|-------------------|------------------|-------------|
| Percolation            | 1.8747(2)         | 0.528(15)        | 1.985(13)   | 0.632(11) |
| Spontaneous \(Z_2\) Breaking | 1.8735(4)     | 0.523(12)        | 1.953(18)   | 0.630(14) |
| Ising Model \[12\]    | 0.518(7)         | 1.970(11)        | 0.6289(8)   |

Table 1: Parameters for percolation and spontaneous \(Z_2\) breaking in 3+1 SU(2).

We therefore conclude that color deconfinement in SU(2) gauge theory can be considered either as spontaneous \(Z_2\) symmetry breaking or as the onset of Polyakov loop percolation. Both phenomena occur at the same critical temperature \(T_c\) and are described in terms of the same set of critical exponents.

3. Percolation in Non-Critical Thermal Systems

We would like to formulate a percolation description of deconfinement in full QCD with dynamical quarks; again we start with a preliminary study and consider spin systems with
a non-vanishing external field \( H \neq 0 \). The basic issue here is to generalize the FK bond weights to include a dependence on \( H \): \( p_b(T, H) \). This problem is not yet solved; we shall address two closely related questions.

Consider the 2-d Ising model with \( H \neq 0 \); the behavior of the magnetization was shown in Fig. 1. Included there is the Kertész line \( T_p(H) \), separating the percolating (\( T \leq T_p(H) \)) and the non-percolating region (\( T > T_p(H) \)). In addition, one can also consider the pseudocritical line \( T_\chi(H) \), defined by the temperature value for which the isothermal susceptibility \( \chi_T \equiv (\partial m/\partial H)_T \) peaks for a given \( H \); for \( H = 0 \), it would diverge at \( T_c \).

We want to compare these two temperature lines [13]; in all percolation calculations, we use the conventional (\( H \)-independent) FK bond weights introduced in section 1. In terms of the reduced variables \( t \equiv (T - T_c)/T_c \) and \( h \equiv H/J \) we find for small \( h \)

\[
t_\chi = c_1 h^{1/\delta} \quad \text{and} \quad t_p = c_2 h^x,
\]

for the pseudocritical Ising line and the Kertész line, respectively, with constants \( c_1 \) and \( c_2 \). For the Ising model, one has the exact result \( 1/\delta = 8/15 \approx 0.533 \), while a numerical study of percolation gives \( x = 0.534(3) \). For small \( h \), the two lines thus have the same \( h \)-dependence. However, \( c_1 \neq c_2 \), so that the lines do not coincide. For large \( h \), this is obvious: \( t_p(h) \to t_b \) for \( h \to \infty \), where \( t_b \) is the bond percolation temperature, but \( t_\chi \to \infty \) for \( h \to \infty \), although the susceptibility peak becomes arbitrarily weak in this limit. This illustrates the necessity to obtain field-dependent bond weights \( p_b(T, H) \) for a reasonable description at \( H \neq 0 \). We note here that a comparison with the pseudocritical behavior of the isothermal susceptibility is not a unique way to specify \( p(T, H) \), since other susceptibilities or the correlation length lead to slightly shifted peak temperatures.

In a second study [14], we consider the 3-d 3-state Potts model, which shows a first order phase transition for \( H = 0 \). When an external field is turned on, the discontinuity in e.g. the magnetization decreases but continues for \( 0 \leq H < H_0 \), defining a line \( T_{\text{dis}}(H) \). This ends for some value \( H = H_0 \) at \( T_c(H_0) \) with a second order phase transition which appears to be in the universality class of the Ising model [14]. For \( H > H_0 \), the partition function is analytic and there is no more thermal critical behavior (see Fig. 2). Using the conventional FK bond weights \( p(T) = 1 - \exp\{-2J/T\} \), we now study the percolation behavior of the model. The result is

- for \( 0 \leq H < H_0 \), there is a discontinuous onset of percolation at the same \( T_{\text{dis}}(H) \) at which there is discontinuous thermal behavior;
- at \( H = H_0 \), the percolation and the thermal transition become continuous and occur at the same temperature \( T_c(H_0) \). In contrast to the Ising-like thermal behavior, the percolation transition leads to exponents which are neither in the Ising nor in the random percolation universality class. This is presumably due to the infinite correlations at \( T_c(H_0) \), similar to what is found for pure site percolation in the 2-d Ising model at the Curie point [14].

Thus again there seems to exist a definite relation between percolation and thermal critical behavior, but with the conventional FK weight, there is not real equivalence; a bond weight \( p(T, H) \) seems to be needed. Here, however, in contrast to the pseudocritical line(s), the problem is well-defined: what \( p(T, H) \) will put percolation at \( T_c(H_0) \) into the Ising universality class? This is quite similar to the original question of what \( p(T) \)
would change random percolation enough to map the new clustering pattern onto thermal critical behavior, solved by the FK bond weights. If a correct $p(T, H)$ can be determined, one would have full equivalence between percolation and thermal critical behavior both in the first order region and for the continuous transition at the endpoint; beyond that, percolation only would persist. Given such a framework, one could then try to address the similar structure in full QCD (Fig. 2).

4. Outlook

From what we have seen, thermal critical behavior can in many cases be formulated as cluster percolation. The interesting feature is, however, that percolation can persist even when thermal critical behavior stops, such as in spin systems with external field. Here the percolation strength $P(T)$ and the cluster size $S(T)$ remain singular when the partition function $Z(T)$ becomes analytic. This raises some intriguing questions. Can one give a more general definition of critical behavior, such that percolation is included? What physical features distinguish the percolating from the non-percolating phase [17]? Is it possible to define a more ‘detailed’ partition function $Z(T, x)$ at some fixed connectivity measure $x$, which results in the usual $Z(T)$ after summation or integration over all $x$? It seems that all these points could eventually provide a new opening to thermodynamics.

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