Cluster Percolation and First Order Phase Transitions in the Potts Model

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Abstract:

The q-state Potts model can be formulated in geometric terms, with Fortuin-Kasteleyn (FK) clusters as fundamental objects. If the phase transition of the model is second order, it can be equivalently described as a percolation transition of FK clusters. In this work, we study the percolation structure when the model undergoes a first order phase transition. In particular, we investigate numerically the percolation behaviour along the line of first order phase transitions of the 3d 3-state Potts model in an external field and find that the percolation strength exhibits a discontinuity along the entire line. The endpoint is also a percolation point for the FK clusters, but the corresponding critical exponents are neither in the Ising nor in the random percolation universality class.

1. Introduction

It is quite well established today that thermal features of physical systems can in many cases be described through the structural properties of connected geometric objects, or clusters. This mapping between thermal aspects of the given model and the geometrical properties of the clusters turns out to be particularly fruitful for the study of the critical behaviour of such models. The increase of the correlation length near the critical point is paralleled by the increase of the average cluster radius, and its divergence to the formation of an infinite cluster. Percolation theory [1, 2] is the natural framework to study the properties of cluster-like structures of a system.

One of the most basic results in this field [3] shows that the q-state Potts model (without external field) can be mapped onto a geometric model: spin configurations become FK cluster configurations by connecting nearest-neighbouring spins of the same orientation with a bond probability \( p_B = 1 - \exp(-J/kT) \), where \( J \) is the Potts spin-spin coupling. The mapping is one to one, so that any statement about thermal properties of the model can be equivalently expressed in terms of cluster quantities. In particular, the magnetization transition is equivalent to the percolation transition of FK clusters, a result originally proved for \( q = 2 \) (Ising model) [4] and subsequently extended [5] to any Potts model which undergoes a second order phase transition. We recall that the Potts model leads to continuous transitions only for \( q = 2, 3, 4 \) in two dimensions and for \( q = 2 \) also in three and higher dimensions.
The FK transformation is, however, independent of the number \( q \) of different spin states of the model. In particular, it remains valid as well in those cases in which the model exhibits a first order phase transition. It is thus natural to ask whether one can establish a relation between the behaviour of FK clusters and the thermal properties of the system also for discontinuous phase changes. In this case, a first order transition persists in the presence of an external field \( H \), as long as \( H \) remains smaller than some critical value \( H_c \). So for \( 0 \leq H < H_c \), there is a whole line of first order phase transitions in the phase diagram of the model. For \( H = H_c \), the transition becomes second order and the critical exponents are conjectured to belong to the Ising universality class; for \( H > H_c \), the partition function becomes analytic and one has at most a rapid crossover.

We note that the equivalence of the thermal and the percolation description provided by the FK transformation is valid only for the case \( H = 0 \). The presence of an external field can in principle be taken into account by introducing a “ghost spin” connected to all the normal spins of the system [8]; the resulting clusters then differ from those defined in [3]. Nevertheless, the usual FK clusters show a number of non-trivial features also in the presence of an external field [9]-[11].

Here we want to study by means of Monte Carlo simulations the behaviour of the FK clusters near the line of first order phase transitions of the 3-dimensional 3-state Potts model. This model has been investigated quite extensively, since its phase transition is closely related to the deconfinement transition of finite temperature QCD [6]. It exhibits a weak first order phase transition for \( H = 0 \), which disappears already for quite small values of the external field. The line of first order phase transitions of this model was recently studied in detail [7], and the position of the endpoint was determined with great precision. In what follows we shall exploit the results of this investigation.

2. The Fortuin-Kasteleyn Transformation and Percolation Variables

The ferromagnetic \( q \)-state Potts model is defined by the Hamiltonian

\[
\mathcal{H} = J \sum_{ij} (1 - \delta_{\sigma_i \sigma_j}) - H \sum_i \delta_{\sigma_i \sigma_h}
\]

where \( J > 0 \) is the spin-spin coupling and \( H \) the external field; the \( \sigma \)'s represent the spin variables of the model and can take on \( q \) different values. The direction of the external field is specified by the spin variable \( \sigma_h \). The partition function \( Z \) is given by

\[
Z(T, H) = \sum_{\sigma} \exp \left[ -\frac{\mathcal{H}(\sigma)}{kT} \right],
\]

with the sum over all spin configurations. By distributing randomly bonds with probability \( p_B \) between all pairs of nearest neighbour sites in the same spin state, one can rewrite \( Z(T, H = 0) \) in the form

\[
Z = \sum_n \left[ \prod_{<ij>, n_{ij} = 1} p_B \prod_{<ij>, n_{ij} = 0} (1 - p_B) q^{c(n)} \right].
\]

Here the sum runs over all bond configurations \( \{ n \} \) (\( \{ n_{ij} = 1 \} \): active bond, \( \{ n_{ij} = 0 \} \): no bond), and \( c(n) \) is the number of FK clusters of the configuration. We stress that in
Eq. (3) the spins of the system do not appear; the partition function is given entirely in terms of bond configurations.

In this work we are mainly interested in the percolation transition of the FK clusters. We therefore first recall the relevant variables. The order parameter is the percolation strength $P$, defined as the probability that a randomly chosen site belongs to an infinite cluster. The analogue of the magnetic susceptibility is the average cluster size $S$,

$$S \equiv \frac{\sum s n_s s^2}{\sum s n_s s},$$

where $n_s$ is the number of clusters of size $s$; the sums exclude the percolating cluster.

For thermal second order phase transitions it is found that near the critical temperature $T_c$,

$$P \sim (T_c - T)^\beta, \quad T \leq T_c;$$

$$S \sim |T - T_c|^{-\gamma}$$

where $\beta$ and $\gamma$ are the critical exponents for the magnetization and the susceptibility, respectively.

To study the percolation transition it is helpful to define also the percolation cumulant. It is the probability of reaching percolation at a given temperature and lattice size, i.e., the fraction of ”percolating” configurations. This variable has two remarkable properties:

- if one plots it as a function of $T$, all curves corresponding to different lattice sizes cross at the same point, which marks the threshold of the percolation transition;
- the percolation cumulants for different values of the lattice size $L$ coincide, if considered as functions of $[(T - T_c)/T_c]L^{1/\nu}$.

These two features allow a rather precise determination of the critical point already from simulations of the system for two different lattice sizes. In general, it is preferable to utilize several lattices in order to evaluate finite size effects and eventual corrections to scaling. Moreover, by using lattices of very different sizes, the scaling of the curves leads to a more precise estimate of the critical exponent $\nu$.

3. Results

We have performed Monte Carlo simulations of the 3d 3-state Potts model for several lattice sizes (40$^3$, 50$^3$, 60$^3$, 70$^3$) and for different values of the parameters $\beta = J/kT$ and $h = H/kT$, using the Wolff cluster update extended to the case of a non-vanishing external field [12]. To identify the clusters of the different configurations, we used the algorithm of Hoshen and Kopelman [13]. We have always adopted free boundary conditions and assumed that a cluster percolates if it connects each pair of opposite faces of the lattice. At each iteration, we measured the energy $E$ of the system, the magnetization $M$, the percolation strength $P$, the average cluster size $S$ and the size of the largest cluster. We recall that the magnetization is the fraction of spins pointing in the direction of the external field. In the case of vanishing field, the majority spin state of the configuration defines the magnetization: $M$ is given by the fraction of the sites in such spin state. We have also measured the size of the largest cluster because it allows us to calculate the
fractal dimension $D$ of the percolating cluster at the critical point. Although the Wolff algorithm is in general very efficient, we were forced to perform many updates between consecutive measurements to reduce appreciably the correlations of the corresponding configurations. In order to get independent configurations for the percolation variables, we have taken up to 1000 updates for the $70^3$ lattice, which made the data production rather slow.

For the analysis near the threshold it turns out to be useful to plot the time history of $M$ and $P$. For a first order phase transition, because of the finite size of the lattice, the system tunnels from one phase to the other, which is the lattice realization of the coexistence of the two phases of the system. This can allow a visual check of the order of the percolation transition.

In general, we expect that a step in the magnetization is accompanied by a step in the average size of the magnetic domains of the system, and consequently by a step of the FK cluster size as well. It is thus natural to expect discontinuous variations of the percolation variables at some threshold. However, the relation between the thermal and the geometric thresholds is not \textit{a priori} evident. There are, in principle, three possible scenarios:

- The configurations of FK clusters percolate at a temperature $T_p$ above $T_c$ ($\beta_p < \beta_c$), and the percolation transition is continuous with critical exponents; unrelated to this transition, both $P$ and $S$ then make a jump at $T_c$ (Fig.1a).

- The configurations of FK clusters percolate at a temperature $T_p$ below $T_c$ ($\beta_p > \beta_c$), and the percolation transition is continuous with critical exponents; unrelated to this transition, only $S$ makes a jump at $T_c$, since $P = 0$ there (Fig.1b).

- The configurations of FK clusters percolate at $T_c$; the percolation transition is discontinuous and both $P$ and $S$ make a jump at $T_c$. In particular, $P$ jumps at $T_c$ from zero to a non-zero value and is still an order parameter (Fig.1c).

For $h = 0$, renormalization group arguments suggest that the third alternative is the correct one, at least in two dimensions ($q > 4$) \[\Box\]. What happens in the presence of an
external field is so far not known. Therefore we will present separately our results for $h = 0$ and $0 < h < h_c$.

3.1 The Case $h=0$

For the model without an external field, the magnetization $M$ is the order parameter of the thermal transition. By studying the time history of $M$ at $T_c$, we observe a tunneling between zero and a non-zero value.

![Figure 2: Time history at the transition point for the magnetization $M$ and the percolation strength $P$ of FK clusters in the 3d 3-state Potts model without external field. The lattice size is $70^3$.](image)

In Fig. 2 we show the magnetization $M$ and the percolation strength $P$ as a function of the number of iteration for a $70^3$ lattice at $\beta_c$. Here we have taken $\beta_c = 0.550565$, as determined in [14]. We see that $P$ follows the variations of $M$; the step of $P$ is somewhat larger and the two "geometric phases" are clearly visible. In particular, we notice that the system passes from a non-percolating phase to a percolating one, as conjectured in [5]. Since the definition of percolation is sharp (either there is a percolating cluster or there is none), we obtain almost always $P = 0$ when the system is in the non-percolating phase. In contrast, the magnetization varies smoothly in the lattice average and hence shows significant fluctuations also in the paramagnetic phase. Hence $P$ can resolve eventual discontinuities due to different phases better than $M$ can.

To check whether this behaviour of the percolation strength is general, we repeat our analysis for the 2d 5-state Potts model. In two dimensions the critical temperature is
given by the exact formula $\beta_c(q) = \log(1 + \sqrt{q})$; which for $q = 5$ yields $\beta_c(5) = 1.174359$. Fig. 3 shows the time history of $M$ and $P$ at $\beta_c(5)$: the result is the same as before.

![Figure 3: Time history at the transition point for the magnetization $M$ and the percolation strength $P$ of FK clusters for the 2d 5-state Potts model without external field. The lattice size is $200^2$.](image)

3.2 The Case $0 < h < h_c$

In the presence of an external field, the magnetization is different from zero at any temperature, so that it is no longer a genuine order parameter for a thermal transition. Nevertheless, for $0 < h < h_c$, $M$ shows discontinuous behaviour at some critical temperature $T_c(h)$, and hence it remains interesting to compare again the behaviour of $M$ and $P$ for $h \neq 0$ along the line of discontinuity $T_c(h)$. This line ends at a critical value of the field, at which the thermal transition becomes continuous; for the 3d 3-state Potts model, $h_c = 0.000775(10)$ (see [4]). In [3], several points of the line of first order phase transitions of the model were determined as well. We choose two of these points, corresponding to the values 0.0005 and 0.0006 of the reduced field $h$, and there determine the time history of $M$ and $P$; it is shown in Figs. 4 and 5, respectively.

From these figures we see that there still are two phases, represented by the two bands of the magnetization values, although now $M$ is never zero. The step between the two bands is narrower for $h = 0.0006$, as it should be, since we are approaching the critical value $h_c$ of the field, at which there would be a continuous variation of $M$. In both cases,
Figure 4: Time history at the transition point and with field $h = 0.0005$ for the magnetization $M$ and the percolation strength $P$ of FK clusters. The lattice size is $70^3$.

Figure 5: Time history at the transition point and with field $h = 0.0006$ for the magnetization $M$ and the percolation strength $P$ of FK clusters. The lattice size is $70^3$. 
the percolation strength also makes a jump from zero to a non-zero value, as we had found for \( h = 0 \). We notice that the number of ‘intermediate’ \( P \) values between the two bands increases when one passes from \( h = 0.0005 \) to \( h = 0.0006 \), which indicates that the transition from one geometrical phase to the other is getting smoother: we are therefore approaching a continuous percolation transition as well.

### 3.3 The Case \( h = h_c \)

The line of first order phase transitions terminates with a continuous phase transition at \( T_c(h_c) \). All thermal variables vary continuously or diverge at this critical point. In particular, the magnetization varies continuously here, and the critical exponents at \( T_c(h_c) \) put the transition into the universality class of the 3d Ising model. The continuous thermal transition suggests that also the percolation transition of the FK clusters becomes continuous at \( h = h_c \). Nevertheless, there are in principle three possible scenarios for the percolation transition:

- The FK clusters percolate at a temperature \( T_p \neq T_c(h_c) \); in this case, due to the finite correlation length of the thermal system at any \( T \neq T_c(h_c) \), the critical percolation exponents will belong to the universality class of random percolation in three dimensions.

- The configurations of FK clusters percolate at \( T_c(h_c) \), but the exponents do not coincide with the ones of the 3d Ising model, which govern the thermal transition at this point.
The configurations of FK clusters percolate at $T_c(h_c)$, and the exponents are the 3d Ising exponents.

We have seen so far that the threshold of the (first order) percolation transition coincides with the (first order) thermal threshold from $h = 0$ up to $h = 0.0006$: that suggests that also for $h = h_c = 0.000775$, the two critical points coincide.

To check if this is indeed correct, we plot in Fig. 6 the percolation cumulant defined in Section 2 as a function of $\beta$ for different lattice sizes. We see that within errors the lines cross at the same point. The vertical dashed lines of the figure mark the thermal threshold determined in [7] within one standard deviation. The agreement between percolation and thermal critical temperatures is very good, particularly if we take into account that we performed our simulations for $h_c = 0.000775$, even though the value of the critical field $h_c$ also contains some uncertainty.

From Fig. 6 we also obtain first indications of the critical exponents of the percolation transition. The height of the crossing point is a universal number, i.e., it identifies a universality class. In our figure, the horizontal lines shown correspond to the universality classes of the 3d Ising model and 3D random percolation (see [15]). The crossing point does not fall on either of the two lines, which means that the percolation exponents of our transition coincide neither with the 3d Ising exponents nor with the exponents of random percolation.

Using standard finite size scaling techniques, we obtain the following values for the critical percolation exponents: $\beta/\nu = 0.32(3)$, $\gamma/\nu = 2.32(2)$, $\nu = 0.45(3)$. From the scaling of the size of the largest cluster at $T_c$ we find that the fractal dimension $D$ of the percolating cluster is $D = 2.66(3)$. It is easy to check the our values satisfy the scaling relations

$$\frac{\gamma}{\nu} + 2\frac{\beta}{\nu} = d, \quad \frac{\gamma}{\nu} + \frac{\beta}{\nu} = D,$$

within the errors we have determined; here $d$ is the space dimension of the lattice. However, the critical indices we have found differ from the Ising ($\beta/\nu = 0.5187(14)$, $\gamma/\nu = 1.963(7)$, $\nu = 0.6294(10)$) and from the random percolation exponents ($\beta/\nu = 0.477(2)$, $\gamma/\nu = 2.045(10)$, $\nu = 0.8765(17)$), as expected. The fact that our exponents do not coincide with the random percolation exponents is in fact a further proof that the geometrical transition takes place exactly at the thermal threshold, because only the presence of an infinite correlation length can shift the values of the critical indices out of the random percolation universality class.

4. Conclusions

We have shown that FK clusters reveal interesting complementary critical features also for spin models undergoing a first order phase transition. In particular, we find that for the 3d 3-state Potts model, the percolation strength jumps from zero to a non-zero value for any value of the external field up to the endpoint. Therefore, the line of thermal first order phase transitions is also a line of first order percolation transitions for the FK clusters, and the percolation strength constitutes a genuine order parameter for any $0 \leq h < h_c$, in contrast to the magnetization. For $h = h_c$, the percolation transition becomes continuous, and its threshold coincides with the thermal critical point. However, the critical indices of the geometrical transition are not in the 3d Ising universality class.
The value of $D$ we have found is bigger than the fractal dimension of the percolating FK cluster in the 3d Ising model ($D_{\text{Ising}} = 2.48(2)$); hence the FK clusters seem too large to define correctly the thermal critical behaviour of the model at the endpoint. This is reminiscent of the situation encountered for the pure site clusters of the 2d Ising model, which reproduce the right critical temperature [13] but not the exponents [17]. In that case the introduction of the bond probability $p_B$ reduces the size of the clusters and restores the correct critical behaviour. We thus conclude that also in our case one has to define a correct bond probability $p_B(J, H, T)$ to obtain a coincidence of thermal and percolation transitions.

In this work, we have limited ourselves to the 3d 3-state Potts model, mainly because here the endpoint is known precisely. As mentioned in Section 3, much computer time is needed to obtain uncorrelated configurations, and hence it would have been very time-consuming to investigate further systems. Nevertheless, it would be of interest to check whether the results we have found are valid for any Potts model which undergoes a first order phase transition for $h = 0$.

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References

[1] D. Stauffer, A. Aharony, *Introduction to Percolation Theory*, Taylor & Francis, London 1994.
[2] G. R. Grimmett, *Percolation*, Springer-Verlag, 1999.
[3] P. W. Kasteleyn, C. M. Fortuin, J. Phys. Soc. of Japan 26 (Suppl.), 11 (1969); C. M. Fortuin, P. W. Kasteleyn, Physica 57, 536 (1972); C. M. Fortuin, Physica 58, 393 (1972); C. M. Fortuin, Physica 59, 545 (1972).
[4] A. Coniglio, W. Klein, J. Phys. A 13, 2775 (1980).
[5] A. Coniglio, F. Peruggi, J. Phys. A 15, 1873 (1982).
[6] B. Svetitsky, L. G. Yaffe, Phys. Rev. D 26, 963 (1982).
[7] F. Karsch, S. Stickan, Phys. Lett. B 488, 319 (2000).
[8] R. H. Swendsen, J. S. Wang, Physica A 167, 565 (1990).
[9] J. Kertész, Physica A 161, 58 (1989).
[10] J. Adler, D. Stauffer, Physica A 175, 222 (1991).
[11] S. Fortunato, H. Satz, Phys. Lett. B 509, 189 (2001).

[12] I. Dimitrović et al., Nucl. Phys. B 350, 893 (1991).

[13] J. Hoshen, R. Kopelman, Phys. Rev. B 14, 3438 (1976).

[14] W. Janke, R. Villanova, Nucl. Phys. B 489, 679 (1997) and references therein.

[15] S. Fortunato, PhD thesis, Bielefeld University, hep-lat/0012006.

[16] A. Coniglio et al., J. Physics A 10, 205-218 (1977).

[17] M. F. Sykes, D. S. Gaunt, J. Phys. A 9, 2131-2137 (1976).