# Theory of continuum percolation I. General formalism

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**Abstract**

The theoretical basis of continuum percolation has changed greatly since its beginning as little more than an analogy with lattice systems. Nevertheless, there is yet no comprehensive theory of this field. A basis for such a theory is provided here with the introduction of the Potts fluid, a system of interacting $s$-state spins which are free to move in the continuum. In the $s \to 1$ limit, the Potts magnetization, susceptibility and correlation functions are directly related to the percolation probability, the mean cluster size and the pair-connectedness, respectively. Through the Hamiltonian formulation of the Potts fluid, the standard methods of statistical mechanics can therefore be used in the continuum percolation problem.

# 1 Introduction

The theoretical basis of continuum percolation [1] changed drastically during the 1970's. In their seminal 1970 paper, Scher and Zallen [2] considered continuum percolation as an extension of lattice models. Noting that the critical volume $\phi_c$ is approximately universal, *i. e.*, essentially independent of the lattice structure, they suggested it might be carried over into continuum systems.

Such a view of the continuum as the representation of what is lattice-independent sits well with the ideas of the renormalization group where the continuum often represents merely a scale at which the underlying lattice blurs and vanishes.

Yet continuum percolation turned out to be much richer than suggested by this conception. In the first extensive simulations of continuum systems, Pike and Seager [3] found that while the critical volume concept works fairly well for spherical objects, it fails completely when the system contains elongated bodies. This and similar works [4] prompted Balberg et al. [5] to suggest that rather than the critical volume, the proper universal quantity might be a critical *excluded* volume. This concept, however, cannot be reduced to some underlying lattice structure. Instead, it requires considering the continuum as fundamental rather than a large scale approximation.

Fruitful as the excluded volume concept was, it nevertheless had clear limitations, since the critical excluded volume is not in fact a truly universal quantity. The shape of the objects in the system clearly influenced the critical point – *i. e.*, the critical density, $\rho_c$, at which an infinite cluster first appears – in a complicated way.

In 1977, Haan and Zwanzig [6] managed to push to its limits the analogy between continuum and lattice percolation. Relying heavily on graph theory, they managed to expand the mean cluster size, $S$, in powers of the density. From this, they obtained values for the critical density which were in good quantitative agreement with the results of simulations. However, this line of developments was reaching its limits as it became clear that continuum percolation could be a complex interplay involving not only the shape of objects – which determined the binding criterion – but also possible interactions between these objects [7]. This new element was beyond accommodation into the analogy with lattice models.

The breakthrough which gave continuum percolation an independent theoretical basis came in two papers by Coniglio et al. [8]. Building on previous work by Hill [9], these researchers showed that the mean cluster size could be related to a pair-connectedness function which had an expansion in powers of the density. This expansion included naturally the interactions. Originally, Coniglio et al. developed this expansion in the context of physical clustering in a gas, but it was soon extended by analogy to other systems [10, 11]. Although the results were mainly qualitative at first, some recent calculations have obtained quantitatively good agreement with simulations [12].

In spite of these successes, the theoretical basis of continuum percolation is still incomplete. The theory of Coniglio et al. suffers from two essential problems. The first is formal. The fundamental quantity in this theory is the pair-connectedness function, yet the only mathematical definition of it is in terms of a power expansion. This is an unsatisfactory situation. Some non-perturbative scheme must underly such a result, but it is absent from the work of Coniglio et al.. Another unsatisfactory aspect is that the extension of this work to various percolation systems has to be done by analogy and reasonable assumption. While this is not a serious problem, one would like to see a more formal basis for such uses. The second main problem is that the theory of Coniglio et al. does not say anything about the order parameter, the percolation probability. This problem is related to the first because perturbative expansions are limited to the region of densities below the critical point, while the order parameter is non-trivial only at densities above this point. Furthermore, the percolation probability is not obtainable from the pair-connectedness, and requires therefore a new approach.

Such limitations also prevent one from approaching some fundamental questions. First among these, probably, is related to the continuum percolation universality class. Computer simulations suggest that continuum percolation belongs to the universality class of lattice percolation. One would like to understand this from the theoretical point of view, as well as to assess whether this is true for all possible interactions and binding criteria. Computer simulations are inadequate to address this problem since they are greatly complicated by the presence of interactions. Furthermore, obtaining critical exponents from a simulation is a notoriously delicate procedure, and one cannot claim yet that the universality class of continuum percolation is known with certainty.

The present series of papers is meant to be the basis for a more comprehensive theory of continuum percolation, which is based on an extension of the classic mapping between the Potts model and lattice percolation which was invented by Kasteleyn and Fortuin [13]. The present extension includes an off-lattice version of the Potts model which I have called the Potts fluid. The $s$-state Potts fluid is introduced in section 2. I show then that, as in the lattice case, all statistical averages in the percolation model may be expressed as averages in the Potts fluid. In section 3, this mapping is applied to the Potts magnetization and susceptibility. The limit $s \to 1$ of these quantities yields the percolation probability, $P(\rho)$, and the mean cluster size, $S$, respectively. Section 4 is concerned with the Potts correlation functions. The pair-connectedness is shown to be directly related to the Potts pair-correlation function. Section 5 sums up the results.

## 2 General formalism

By "continuum percolation" I always mean a system of particles interacting through a pair potential $v(\vec{r}_i, \vec{r}_j)$ and obeying classical statistical mechanics. In addition to their interaction, the particles possess another property, "the connectivity", determined by a probability function $p(\vec{r}_i, \vec{r}_j)$ which is the probability that two particles located at $\vec{r}_i$ and $\vec{r}_j$ are bound, or connected, to each other. A *cluster* is a group of such connected particles. Let us also define $q(\vec{r}_i, \vec{r}_j) = 1 - p(\vec{r}_i, \vec{r}_j)$ as the complementary function.

Note that we do not assume any "locking" mechanism: bound particles do not remain glued together thereafter. Indeed, the system does not evolve with time at all. The point of view adopted here is that of equilibrium statistical mechanics, where all properties are derived from an ensemble of "snapshot" configurations. As a result, the properties of connectivity and interaction are arranged hierarchically. The interaction alone determines the configuration of the particles, which in turn helps determine the connectivity, but the connectivity does not in its turn influence the configuration.

Often, as in systems of permeable objects [3], $p(\vec{r}_i, \vec{r}_j)$ takes only two values, 0 or 1, but no such restrictions are assumed here. Thus, the connectivity state need not be uniquely determined by the geometrical configuration of the particles. Only its probability distribution is fully determined through the function $p(\vec{r}_i, \vec{r}_j)$.

The formalism presented here is an extension of the Kasteleyn-Fortuin mapping between lattice percolation and the Potts model [13]. For the continuum case I will define an extension of the Potts model hereafter called the *Potts fluid*.

The $s$-state Potts fluid is a system of N "spins" $\{\lambda_i\}_{i=1}^N$ each having $s$ possible states, and obeying classical statistical mechanics. Each spin has a position $\vec{r}_i$ in the continuum and the spins interact with each other through a spin-dependent pair potential $V(\vec{r}_i, \lambda_i; \vec{r}_j, \lambda_j)$, such that

$$V(\vec{r}_i, \lambda_i; \vec{r}_j, \lambda_j) \equiv V(i,j) = \begin{cases} U(\vec{r}_i, \vec{r}_j) & \text{if} \quad \lambda_i = \lambda_j \\ W(\vec{r}_i, \vec{r}_j) & \text{if} \quad \lambda_i \neq \lambda_j \end{cases} \tag{2.1}$$

where $U$ and $W$ are arbitrary functions.

The spins may also couple to an external field $h(\vec{r})$ which tends to align them in some given state. If we arbitrarily denote this state as "1" , then the interaction Hamiltonian is

$$H_{int} = -\sum_{i=1}^{N} \psi(\lambda_i) h(\vec{r}_i) \tag{2.2}$$

where

$$\psi(\lambda) = \begin{cases} s-1 & \text{if} \quad \lambda = 1 \\ -1 & \text{if} \quad \lambda \neq 1 \end{cases} \tag{2.3}$$

For conciseness, two spins in the same state will be said to be *parallel* to each other (though the state need not actually correspond to any spatial directions). Two spins in different states will be called non-parallel.

As in all classical systems [14], the dependence on the momenta can be factored out so that all statistical averages depend on the configuration integral

$$Z = \frac{1}{N!} \sum_{\{\lambda_m\}} \int d\vec{r}_1 \cdots d\vec{r}_N \, \exp\left[ -\beta \sum_{i>j} V(i,j) + \beta \sum_{i=1}^{N} h(i) \psi(\lambda_i) \right] \tag{2.4}$$

where the sum $\sum_{\{\lambda_m\}}$ is over all spin configurations, and $\beta = 1/kT$ is the inverse temperature as usual.

Now, any continuum percolation model defined by $v(i,j)$ and $p(i,j)$ can be mapped onto an appropriate Potts fluid model with a pair-spin interaction defined by

$$\begin{aligned} U(i,j) &= v(i,j) \\ \exp\left[-\beta W(i,j)\right] &= q(i,j) \exp\left[-\beta v(i,j)\right] \end{aligned} \tag{2.5}$$

This mapping relates statistical averages of the Potts fluid to statistical averages of the percolation model. The most fundamental relation is obtained for the Potts fluid configuration integral Eq. (2.4). However, because the following derivation can be a little confusing, let us anticipate the final result. The formal mapping Eq. (2.5) induces a geometrical mapping between spin configurations and connectivity states. To every particle in the percolation system we assign a spin in such a way that if two objects belong to the same cluster in the percolation model, they are assigned the same spin (i.e, their spins are parallel) in the corresponding Potts fluid spin configuration. However, the actual value of this common spin is selected at random. Therefore the mapping from the percolation model to the Potts fluid is one to many. Any connectivity state corresponds to several spin configurations, which differ from one another by the actual value of the spin assigned in common to all the particles in a given cluster. Because of the one to many character of this mapping, the status of two parallel spins differs radically from the status of two non-parallel spins. If two spins are non-parallel, they *must* belong to different clusters in the percolation picture. However, if two spins are parallel *no conclusion* may be drawn as to their connectivity state. They might be parallel because they belong to the same cluster. But they might also belong to different clusters and have been assigned the same spin by chance. Since the common spin of every particle in a cluster is assigned randomly, it is quite probable that two unrelated clusters end up with the same spin. This difference makes "disconnectedness" a more basic property than connectedness in the sense that given a spin configuration, one can never deduce with certainty that two particles belong to the same cluster in the corresponding percolation model. However, one may be able to deduce that two particle *do not* belong to the same cluster.

Let us now see how this geometrical mapping arises naturally out of the formal mapping Eq. (2.5). For simplicity, let us assume temporarily that the external field vanishes, *i. e.*, $h(\vec{r}) = 0$. Introduce the notation

$$\begin{aligned} Z &= \frac{1}{N!} \int d\vec{r}_1 \cdots d\vec{r}_N \, Q(\vec{r}_1, \ldots, \vec{r}_N) \\ Q(\vec{r}_1, \ldots, \vec{r}_N) &= \sum_{\{\lambda_m\}} \exp\left[-\beta \sum_{i>j} V(\vec{r}_i, \vec{r}_j)\right] \end{aligned} \tag{2.6}$$

In the expression for $Q(1, \ldots, N)$, let us separate all possible configurations

$\lambda_m$ into those where $\lambda_1 = \lambda_2$ and the rest

$$\begin{aligned} Q &= e^{-\beta U(1,2)} \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 = \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \\ &+ e^{-\beta W(1,2)} \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 \neq \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \end{aligned} \tag{2.7}$$

where $\sum_{(i,j)-(1,2)}$ means a summation over all pairs $(i, j)$ except the pair $(1, 2)$. In the second term on the l.h.s of Eq. (2.7) we can now rewrite

$$\begin{aligned} \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 \neq \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] &= \sum_{\{\lambda_m\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \\ &- \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 = \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \end{aligned} \tag{2.8}$$

where the sum $\sum_{\{\lambda_m\}}$ is now performed over all spin configurations without constraints. Eq. (2.7) now becomes

$$\begin{aligned} Q &= \left[ e^{-\beta U(1,2)} - e^{\beta W(1,2)} \right] \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 = \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \\ &+ e^{-\beta W(1,2)} \sum_{\{\lambda_m\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \end{aligned} \tag{2.9}$$

The mapping Eq. (2.5) then implies that

$$\begin{aligned} Q &= p(1,2) e^{-\beta v(1,2)} \sum_{\left\{ \substack{\lambda_m \\ \lambda_1 = \lambda_2} \right\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \\ &+ q(1,2) e^{-\beta v(1,2)} \sum_{\{\lambda_m\}} \exp\left[ -\beta \sum_{(i,j)-(1,2)} V(i,j) \right] \end{aligned} \tag{2.10}$$

where we used the fact that $p(1,2) = 1 - q(1,2)$. Repeating this procedure for the pair $(1,3)$, we obtain

$$
\begin{aligned}
Q &= p(1,2)\, p(1,3) e^{-\beta[v(1,2)+v(1,3)]} \sum_{\left\{\substack{\lambda_m \\ \lambda_1=\lambda_2=\lambda_3}\right\}} \exp\left[-\beta \sum_{(i,j)-(1,2)-(1,3)} V(i,j)\right] \\
&+ p(1,2)\, q(1,3) e^{-\beta[v(1,2)+v(1,3)]} \sum_{\left\{\substack{\lambda_m \\ \lambda_1=\lambda_2}\right\}} \exp\left[-\beta \sum_{(i,j)-(1,2)-(1,3)} V(i,j)\right] \\
&+ q(1,2)\, p(1,3) e^{-\beta[v(1,2)+v(1,3)]} \sum_{\left\{\substack{\lambda_m \\ \lambda_1=\lambda_3}\right\}} \exp\left[-\beta \sum_{(i,j)-(1,2)-(1,3)} V(i,j)\right] \\
&+ q(1,2)\, q(1,3) e^{-\beta[v(1,2)+v(1,3)]} \sum_{\{\lambda_m\}} \exp\left[-\beta \sum_{(i,j)-(1,2)} V(i,j)\right] \qquad (2.11)
\end{aligned}
$$

One sees therefore how the geometric mapping comes about. Every sum is performed over a subset of spin configurations determined by a set of *constraints* of the form $\lambda_1 = \lambda_2, \ldots$. All constraints are equalities between spin pairs. There are no constraints forcing two spins to be non-parallel. Every constraint $\lambda_i = \lambda_j$ also brings forth a factor $p(i,j)$, the probability for the pair to be bound. Since a bound pair belongs by definition to the same cluster, we see the beginning of the geometrical mapping in which spins in a single cluster have parallel spins. To see the full mapping, we need to repeat the procedure outlined in Eqs. ( 2.7)-(2.11) for *all* pairs of spins. Let us consider one of the sums into which the function $Q$ has been decomposed a step before, and consider a pair $(m,n)$. Two possibilities arise:

1. Previous constraints already determine that $\lambda_m = \lambda_n$ (for example, there could be some $k$ for which $\lambda_m = \lambda_k$ and $\lambda_n = \lambda_k$). Then, necessarily, $V(m,n) = U(m,n) = v(m,n)$. Hence

$$
\sum_{\left\{\substack{\lambda_m \\ \text{previous} \\ \text{constraints}}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots} V(i,j)\right]
$$

$$
\begin{aligned}
&= e^{-\beta v(m,n)} \sum_{\left\{\substack{\lambda_m \\ \text{previous} \\ \text{constraints}}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots-(m,n)} V(i,j)\right] \\
&= p(m,n)\, e^{-\beta v(m,n)} \sum_{\left\{\substack{\lambda_m \\ \text{prev.} \\ \text{constr.}}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots-(m,n)} V(i,j)\right] \\
&+ q(m,n)\, e^{-\beta v(m,n)} \sum_{\left\{\substack{\lambda_m \\ \text{prev.} \\ \text{constr.}}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots-(m,n)} V(i,j)\right]
\end{aligned}
\tag{2.12}
$$

where we have used $p(m,n) + q(m,n) = 1$.

2. Previous constraints do not determine that $\lambda_m = \lambda_n$. Then the situation is as it was for the pair $(1,2)$, and the sum will split in the following way

$$
\begin{aligned}
&\sum_{\left\{\substack{\lambda_m \\ \text{constr.}}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots} V(i,j)\right] \\
&\quad = p(m,n)\, e^{-\beta v(m,n)} \sum_{\left\{\substack{\lambda_m: \cdots \\ \lambda_m=\lambda_n}\right\}} \exp\left[-\beta \sum_{(i,j)-\cdots-(m,n)} V(i,j)\right] \\
&\quad + q(m,n)\, e^{-\beta v(m,n)} \sum_{\{\lambda_m: \ldots\}} \exp\left[-\beta \sum_{(i,j)-\cdots-(m,n)} V(i,j)\right]
\end{aligned}
\tag{2.13}
$$

From the point of view of the geometrical mapping, case (1) means that $m$ and $n$ already belong to the same cluster by virtue of some other particles which link them (perhaps indirectly). Hence, it doesn't matter whether they are also directly bound to each other [a case which contributes the factor $p(m,n)$] or not [a case which contributes the factor $q(m,n)$]. As a result, both contributions appear without the addition of any constraint. In case

(2) on the other hand, the appearance of the factor $p(m,n)$ also requires a new constraint which now implies that $m$ and $n$ are bound and therefore belong to the same cluster. The factor $q(m,n)$ requires no such constraint, since if the particles belong to different clusters, their spin attribution is random.

When all pairs have been covered, the set of constraints of a particular sum specifies exactly which particles belongs to which clusters in the original percolation model configuration. Since the expression for $Q$ contains sums over all possible constraints, it can be rewritten as a sum over all possible clusterings of the original percolation configuration. Thus, let us define

$$P(\text{ conn.}) \equiv \prod_{\left\{\substack{\text{all}\\ \text{bound}\\ \text{pairs}\\ (i,j)}\right\}} p(i,j) \prod_{\left\{\substack{\text{all}\\ \text{unbound}\\ \text{pairs}\\ (m,n)}\right\}} q(m,n)\ \exp\left[-\beta\sum_{i>j} v(i,j)\right] \tag{2.14}$$

Then we can write $Q$ as

$$Q = \sum_{\left\{\substack{\text{all possible}\\ \text{connectivity}\\ \text{states}}\right\}} \sum_{\left\{\substack{\lambda_m \text{ consistent}\\ \text{with the}\\ \text{connectivity}\\ \text{state}}\right\}} P(\text{ conn.}) \tag{2.15}$$

where the sum over all spins is consistent with the connectivity state in the sense of the geometrical mapping, *i. e.*, that all particles within a single cluster must be assigned the same spin (note, however, that not all particles in a cluster need be *directly* bound to each other).

From the probabilistic interpretation of the functions $p(i,j)$, $q(i,j)$ and of the usual canonical Gibbs distribution, we now see that up to a normalization, Eq. (2.14) means that

$$\begin{aligned} P(\text{ conn.}) \quad \propto \quad & \text{Probability density of finding a configuration}(\vec{r}_1,\ldots,\vec{r}_N) \\ & \text{such that all pairs } (i,j) \text{ are bound and all pairs } (m,n) \\ & \text{are unbound.} \end{aligned} \tag{2.16}$$

Returning now to Eq. (2.4), and restoring the external field $h(\vec{r})$, we finally find

$$Z = \frac{1}{N!}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{ conn.}) \sum_{\{\lambda_m:\ \text{cl}\}} \exp\left[\beta \sum_{i=1}^{N} h(\vec{r}_i)\psi(\lambda_i)\right] \tag{2.17}$$

Here the symbol $\sum_{\{\lambda:\ \text{cl}\}}$ means a sum over all spin configurations consistent with the clustering, *i. e.*, with the connectivity state in the sense of the geometrical mapping.

This expression has the form of an average over all percolation configuration (up to nonimportant normalization factors). It is the fundamental relation between statistical averages calculated in the percolation model and quantities calculated in the corresponding Potts fluid. As we shall see in a moment, it allows us to obtain percolation-related quantities by calculating properties of the Potts fluid defined in Eq. (2.5). However, since there is no equivalent in the percolation model to the field $h$, we need to set this field to zero. In this case, Eq. (2.17) becomes

$$Z = \frac{1}{N!}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{conn.}) \quad s^{N_c} \tag{2.18}$$

where $N_c$ is the total number of clusters in the relevant connectivity state. The term $s^{N_c}$ is then the number of possible assignments of spins to these $N_c$ clusters in accordance with the geometrical mapping.

Finally we shall have to get rid of the free parameter $s$. As in the usual Kasteleyn-Fortuin mapping [13], the interesting case is the limit $s \to 1$. The resulting expression

$$Z_p \equiv \frac{1}{N!}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{conn.}) \tag{2.19}$$

is just the normalization factor required for averages performed within the percolation model. Hence,

$$Z = Z_p \left\langle \sum_{\{\lambda_m:\ \text{cl}\}} \exp\left[\beta \sum_{i=1}^{N} h(\vec{r}_i)\psi(\lambda_i)\right]\right\rangle_p \tag{2.20}$$

where the symbol $\langle\ \rangle_p$ means a canonical average performed in the percolation model, *i. e.*,

$$\langle F(1,\ldots,N)\rangle_p = \frac{1}{N!Z_p}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{conn.})\, F(1,\ldots,N) \quad (2.21)$$

where $F$ is some quantity defined in the percolation model.

Similarly, we need averages performed in the Potts fluid, which will be denoted by $\langle\ \rangle_s$. Given a quantity $G$ defined in the Potts fluid, we have

$$\begin{aligned}\langle G(1,\lambda_1;\ldots;N,\lambda_N)\rangle_s &= \frac{1}{N!Z}\int d1\cdots dN \sum_{\{\lambda_m\}} G(1,\lambda_1;\ldots;N,\lambda_N)\\ &\quad\times\exp\left[-\beta\sum_{i>j}V(i,j)+\beta\sum_{i=1}^{N}h(i)\psi(\lambda_i)\right]\end{aligned} \quad (2.22)$$

Eq. (2.15) now implies that in general, for any quantity $G(1,\lambda_1;\ldots;N,\lambda_N)$ defined in the Potts fluid system, we have that

$$\langle G(1,\lambda_1;\ldots;N,\lambda_N)\rangle_s = \left\langle \sum_{\{\lambda_m:\ \text{cl}\}} G(1,\lambda_1;\ldots;N,\lambda_N)e^{\left[\beta\sum h(i)\psi(\lambda_i)\right]}\right\rangle_p \quad (2.23)$$

This fundamental relation allows us to translate every quantity in the Potts fluid into some quantity defined in the continuum percolation model.

We now turn to using Eq. (2.20) to show that the average magnetization in the Potts fluid is directly related to the order parameter of the percolation model, the percolation probability.

# 3 The Potts magnetization and the percolation probability

The magnetization of the Potts fluid is defined as in the usual Potts model by

$$M = \frac{1}{\beta N(s-1)}\frac{\partial \ln Z}{\partial h} \quad (3.1)$$

where $h$ is the now constant external field. From Eqs. (2.20) and (2.23), we have

$$\begin{aligned} M &= \left\langle \frac{1}{N(s-1)} \sum_{i=1}^{N} \psi(\lambda_i) \right\rangle_s \\ &= \left\langle \frac{1}{N(s-1)} \sum_{\{\lambda_m:\ \mathrm{cl}\}} \left\{ \sum_{i=1}^{N} \psi(\lambda_i) \exp\left[\beta \sum_{i=1}^{N} h(\vec{r}_i)\psi(\lambda_i)\right] \right\} \right\rangle_p \end{aligned} \tag{3.2}$$

In order to calculate this expression, we need to characterize more formally the sum over all spin states. In a given connectivity state, let us denote by $N_r$ $(1 \leq r \leq N)$ the number of clusters containing exactly $r$ particles (possibly $N_r = 0$). Also, because of their particular role, let us denote separately the number of spanning clusters by $N_s$ (as we take $N \to \infty$, $N_s$ is either 0 or 1). Any connectivity state thus corresponds to a set of numbers $(N_1, N_2, \ldots, N_N, N_s)$ (other connectivity states may also correspond to the same set). For a given spin configuration consistent with this clustering, let us denote by $k_r$ the number of $r$-clusters which have been assigned the spin 1 ($k_s$ will represent the spanning clusters assigned the spin 1). Every spin configuration generates therefore a set $(k_1, k_2, \ldots, k_N, k_s)$. Then, the total number of spin configurations consistent with the given clustering is

$$\sum_{k_1=0}^{N_1} \sum_{k_2=0}^{N_2} \cdots \sum_{k_N=0}^{N_N} \sum_{k_s=0}^{N_s} \binom{k_1}{N_1} \cdots \binom{k_N}{N_N} \binom{k_s}{N_s} (s-1)^{N_1-k_1} \cdots (s-1)^{N_s-k_s} \tag{3.3}$$

The factor $(s-1)^{N_r-k_r}$ is the number of possible spin assignments to the $(N_r - k_r)$ $r$-clusters which have a spin different from 1.

Consider now the expression $\sum_{i=1}^{N} \psi(\lambda_i)$. From the definition of $\psi(\lambda)$, Eq. (2.3), every $j$-cluster with a spin 1 contributes a term $j(s-1)$ to this expression. Every $j$-cluster with a spin different from 1 contributes $j(-1)$ to it. Therefore, for a given spin configuration,

$$\begin{aligned} \sum_{i=1}^{N} \psi(\lambda_i) &= (s-1)\left[\sum_{j=1}^{N} jk_j + n_s k_s\right] - \left[\sum_{j=1}^{N} j(N_j - k_j) + n_s(N_s - k_s)\right] \\ &= s\left[\sum_{j=1}^{N_s} jk_j\right] - N \end{aligned} \tag{3.4}$$

where $n_s$ is the number of spins in the spanning cluster (we anticipate the thermodynamic limit and assume that the spanning cluster, if it exists, is unique), and where we have used the identity $\sum_{j=1}^{N_s} jk_j = N$. The notation $\sum_{j=1}^{N_s} jk_j$ is shorthand for $n_s k_s + \sum_{j=1}^{N} jk_j$.

We now have that

$$\begin{aligned}
&\frac{1}{N(s-1)} \sum_{\{\lambda_m:\ \mathrm{cl}\}} \left\{ \exp\left[\beta h \sum_{i=1}^{N} \psi(\lambda_i)\right] \sum_{i=1}^{N} \psi(\lambda_i) \right\} \\
&= e^{-\beta h N} \prod_{l=1}^{N_s} \left\{ \sum_{k_l=0}^{N_l} \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} \right. \\
&\qquad \left. \times \left[ \frac{1}{N(s-1)} \sum_{j=1}^{N_s} (sjk_j) - N \right] \right\} \qquad (3.5)
\end{aligned}$$

where $\prod_{l=1}^{N_s} \equiv \prod_{l=1}^{N_N} \cdots \times (\text{case } l = N_s)$.

It is easy to prove (*e. g.*, by induction) the two identities

$$\sum_{k_l=0}^{N_l} \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} = \left[e^{l\beta hs} + (s-1)\right]^{N_l} \qquad (3.6)$$

$$\sum_{k_l=0}^{N_l} k_l \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} = \frac{\left[e^{l\beta hs} + (s-1)\right]^{N_l}}{e^{l\beta hs} + (s-1)} N_l\, e^{l\beta hs} \qquad (3.7)$$

Therefore,

$$\prod_{l=1}^{N_s} \left[ \sum_{k_l=0}^{N_l} \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} \right] (-N) = -N \prod_{l=1}^{N-s} \left[e^{l\beta hs} + (s-1)\right]^{N_l} \qquad (3.8)$$

and

$$\begin{aligned}
&\prod_{l=1}^{N_s} \left\{ \sum_{k_l=0}^{N_l} k_l \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} \sum_{j=1}^{N_s} js \right\} \\
&= \left[ \prod_{\substack{l=1 \\ l\neq j}}^{N_s} \sum_{k_l=0}^{N_l} \binom{k_l}{N_l} (s-1)^{N_l-k_l} \left(e^{l\beta hs}\right)^{k_l} \right]
\end{aligned}$$

$$\times \sum_{k_j=0}^{N_j} k_j \binom{k_j}{N_j} (s-1)^{N_j-k_j} \left(e^{j\beta hs}\right)^{k_j}$$

$$= \sum_{j=1}^{N_s} sjN_j \frac{e^{j\beta hs}}{e^{j\beta hs}+(s-1)} \prod_{l=1}^{N_s} \left[e^{l\beta hs}+(s-1)\right]^{N_l} \tag{3.9}$$

Combining these two equations, we finally obtain

$$\sum_{\{\lambda_m:\ \mathrm{cl}\}} \left\{ \exp\left[\beta h \sum_{i=1}^{N} \psi(\lambda_i)\right] \sum_{i=1}^{N} \psi(\lambda_i) \right\}$$

$$= e^{-\beta hN} \prod_{l=1}^{N_s} \left[e^{l\beta hs}+(s-1)\right]^{N_l} \left\{ -N + \sum_{j=1}^{N_s} sjN_j \frac{e^{j\beta hs}}{e^{j\beta hs}+(s-1)} \right\} \tag{3.10}$$

Recalling that $N = \sum_{j=1}^{N_s} jN_j$ and rearranging terms, we have that

$$\frac{1}{N(s-1)} \sum_{\{\lambda_m:\ \mathrm{cl}\}} \left\{ \exp\left[\beta h \sum_{i=1}^{N} \psi(\lambda_i)\right] \sum_{i=1}^{N} \psi(\lambda_i) \right\}$$

$$= \frac{1}{N} e^{-\beta hN} \prod_{l=1}^{N_s} \left[e^{l\beta hs}+(s-1)\right]^{N_l} \left\{ \sum_{j=1}^{N_s} jN_j \frac{e^{j\beta hs}-1}{e^{j\beta hs}+(s-1)} \right\}$$

$$= \prod_{l=1}^{N_s} \left[1+(s-1)e^{-s\beta lh}\right]^{N_l} \sum_{j=1}^{N_s} \frac{jN_j}{N} \left[\frac{1-e^{-j\beta hs}}{1+(s-1)e^{-j\beta hs}}\right] \tag{3.11}$$

Hence

$$M = \left\langle \prod_{l=1}^{N_s} \left[1+(s-1)e^{-s\beta lh}\right]^{N_l} \sum_{j=1}^{N_s} \frac{jN_j}{N} \left[\frac{1-e^{-j\beta hs}}{1+(s-1)e^{-j\beta hs}}\right] \right\rangle_p \tag{3.12}$$

To obtain a quantity directly related to the percolation model, we need to take the limit $s \to 1$, which yields

$$M_{(s\to 1)} = \left\langle \frac{1}{N} \sum_{j=1}^{N_s} jN_j - \frac{1}{N} \sum_{j=1}^{N_s} e^{-j\beta h} \right\rangle_p = 1 - \left\langle \frac{1}{N} \sum_{j=1}^{N_s} jN_j e^{-j\beta h} \right\rangle_p \tag{3.13}$$

Finally, we need to take the thermodynamic limit and set the external field to 0. As always, we must be careful in the order of these limits [15]. A broken symmetry state will only be obtained if the field remains finite while $N \to \infty$. In the limit $N \to \infty$, the spanning cluster behaves differently from the finite clusters. Eq. (3.13) can be rewritten as

$$M = 1 - \frac{1}{N}\left\langle \sum_{j=1}^{N} jN_j e^{-j\beta h} + \frac{n_s N_s}{N} e^{-\beta h n_s} \right\rangle_p \tag{3.14}$$

In the limit $N \to \infty$, the factors $\exp(-j\beta h)$ remain finite, but $\exp(-\beta h n_s) \to 0$, because the spanning cluster then becomes infinite. It is this property which distinguishes it from all finite clusters. Hence

$$M = 1 - \lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{j=1}^{N} jN_j e^{-j\beta h} \right\rangle_p \tag{3.15}$$

Finally,we can set $h = 0$. At this stage, the limits commute and we obtain

$$M = 1 - \lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{j=1}^{N} jN_j \right\rangle_p = 1 - \lim_{N\to\infty} \left\langle \frac{N - n_s}{N} \right\rangle_p = \lim_{N\to\infty} \left\langle \frac{n_s}{N} \right\rangle_p \tag{3.16}$$

This is exactly the probability that a particle picked at random belongs to the infinite cluster, which is by definition the percolation probability $P(\rho)$. Therefore,

$$\lim_{h\to 0} \lim_{N\to\infty} \lim_{s\to 1} M = P(\rho) \tag{3.17}$$

and the percolation order parameter is directly calculable from the Potts magnetization.

We can calculate the Potts susceptibility most easily from Eq. (3.15), before we set the field to 0 (it is easy to see that the derivative $\partial/\partial h$ commutes with all the operations performed up to that point). Thus,

$$\chi = \frac{\partial M}{\partial h} = \beta \lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{j=1}^{N} j^2 N_j e^{-j\beta h} \right\rangle_p \tag{3.18}$$

Taking now the limit $h \to 0$ and using again that $N = \sum_{j=1}^{N_s} jN_j$ gives

$$\chi = \frac{\partial M}{\partial h} = \beta \lim_{N\to\infty} \left\langle \frac{\sum_{j=1}^{N} j^2 N_j}{\sum_{j=1}^{N_s} jN_j} \right\rangle_p \tag{3.19}$$

For densities *lower* than the critical density, there is no spanning cluster (in the thermodynamic limit), so that

$$\chi = \beta \lim_{N\to\infty} \left\langle \frac{\sum\limits_{j=1}^{N} j^2 N_j}{\sum\limits_{j=1}^{N} j N_j} \right\rangle_p = \beta S \qquad (\rho < \rho_c) \tag{3.20}$$

where $S$ is the average mean cluster size, by definition [16].

Therefore, we can calculate the percolation probability by calculating instead the magnetization of a corresponding Potts fluid, and the average mean cluster size by calculating the Potts susceptibility.

# 4 Correlation functions

The Potts magnetization and susceptibility are directly related to the $n$-density functions of the Potts fluid, which are defined in analogy to the $n$-density functions of a classical liquid [14] as

$$\rho^{(n)}(\vec{r}_1, \lambda_1; \vec{r}_2, \lambda_2; \ldots, \vec{r}_n, \lambda_n) = \\ \frac{1}{Z(N-n)!} \int d\vec{r}_{n+1} \cdots d\vec{r}_N \, \exp\left[ -\beta \sum_{i>j} V(i,j) - \beta \sum_{i=1}^{N} h(i)\psi(\lambda_i) \right] \tag{4.1}$$

The normalization is chosen so that

$$\sum_{\{\lambda_1,\ldots,\lambda_n\}} \int d1 \cdots dn \; \rho^{(n)} = s^N \frac{N!}{(N-n)!} \tag{4.2}$$

The $n$-density functions can also be expressed as canonical averages,

$$\rho^{(1)}(\vec{x}, \sigma) = \left\langle \sum_{i=1}^{N} \delta(\vec{r}_i - \vec{x})\, \delta_{\lambda_i,\sigma} \right\rangle_s \tag{4.3}$$

$$\rho^{(2)}(\vec{x}, \sigma; \vec{y}, \eta) = \left\langle \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \delta(\vec{r}_i - \vec{x})\, \delta(\vec{r}_j - \vec{y})\, \delta_{\lambda_i,\sigma}\, \delta_{\lambda_j,\eta} \right\rangle_s \tag{4.4}$$

$$\vdots$$

Now, we can rewrite

$$\psi(\lambda_i) = (s-1)\delta_{\lambda_i,1} - \sum_{\lambda\neq 1}\delta_{\lambda_i,\lambda} \tag{4.5}$$

Using the identity $\int d\vec{x}\,\delta(\vec{r}_i - \vec{x}) = 1$, we now have

$$\begin{aligned}
\left\langle \sum_{i=1}^{N}\psi(\lambda_i)\right\rangle_s &= \left\langle (s-1)\sum_{i=1}^{N}\int d\vec{x}\,\delta(\vec{r}_i - \vec{x})\delta_{\lambda_i,1}\right\rangle_s \\
&- \left\langle \sum_{i=1}^{N}\int d\vec{x}\,\delta(\vec{r}_i - \vec{x})\sum_{\lambda\neq 1}\delta_{\lambda_i,\lambda}\right\rangle_s \\
&= \int d\vec{x}\left[(s-1)\rho^{(1)}(\vec{x},\sigma=1) - \sum_{\sigma\neq 1}\rho^{(1)}(\vec{x},\sigma)\right]
\end{aligned} \tag{4.6}$$

Since the field $h$ preserves the symmetry between all the spins $\lambda \neq 1$, $\rho^{(1)}(\vec{x},\sigma)$ must be the same for all $\sigma \neq 1$. Hence,

$$M = \left\langle \frac{1}{N(s-1)}\sum_{i=1}^{N}\psi(\lambda_i)\right\rangle_s = \frac{1}{N}\int d\vec{x}\left[\rho^{(1)}(\vec{x},1) - \rho^{(1)}(\vec{x},\alpha)\right] \tag{4.7}$$

where $\alpha$ denotes some (arbitrary) spin value other than 1. From the normalization, Eq. (4.2),it is now obvious that

$$\begin{aligned}
\int d\vec{x}\,\rho^{(1)}(\vec{x},1) &= n_1 \equiv \text{ number of spins in state 1} \\
\int d\vec{x}\,\rho^{(1)}(\vec{x},\alpha) &= n \equiv \text{ number of spins in any state } \alpha \neq 1
\end{aligned} \tag{4.8}$$

Hence

$$M = \frac{1}{N}(n_1 - n) \tag{4.9}$$

is just the excess density of spins in the state 1 over the density of spins in any other state.

From Eq. (3.2), and the definition $\chi = \partial M/\partial h$, the susceptibility is

$$\chi = \left\langle \frac{\beta}{N(s-1)}\sum_{i\neq j}\psi(\lambda_i)\psi(\lambda_j)\right\rangle_s + \left\langle \frac{\beta}{N(s-1)}\sum_{i=1}^{N}\psi^2(\lambda_i)\right\rangle_s \tag{4.10}$$

Repeating the steps leading to Eq. (4.6), we have

$$\left\langle \frac{\beta}{N(s-1)} \sum_{i=1}^{N} \psi^2(\lambda_i) \right\rangle_s = \frac{\beta}{N(s-1)} \int d\vec{x} \sum_{\sigma} \psi^2(\sigma)\, \rho^{(1)}(\vec{x},\sigma) \tag{4.11}$$

where the sum over $\sigma$ runs over all the $s$ possible spin states.

On the other hand,

$$\sum_{i\neq j} \psi(\lambda_i)\psi(\lambda_j) = \sum_{\alpha}\sum_{\gamma} \psi(\alpha)\psi(\gamma) \sum_{i\neq j} \delta_{\lambda_i,\alpha}\delta_{\lambda_j,\gamma} \tag{4.12}$$

where, again, the sum over $\alpha$ and $\gamma$ runs over the $s$ spin states. Hence, by a derivation similar to the one used for Eq. (4.6), we have

$$\begin{aligned} &\left\langle \sum_{i\neq j} \psi(\lambda_i)\psi(\lambda_j) \right\rangle_s \\ &= \left\langle \sum_{\alpha}\sum_{\gamma} \psi(\alpha)\psi(\gamma) \sum_{i\neq j} \int d\vec{x}\, d\vec{y}\; \delta(\vec{r}_i - \vec{x})\, \delta(\vec{r}_j - \vec{y})\, \delta_{\lambda_i,\alpha}\, \delta_{\lambda_j,\gamma} \right\rangle_s \\ &= \int d\vec{x}\, d\vec{y} \left[ \sum_{\alpha}\sum_{\gamma} \psi(\alpha)\psi(\gamma)\, \rho^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \right] \end{aligned} \tag{4.13}$$

Therefore

$$\begin{aligned} \chi &= \frac{\beta}{N(s-1)} \int d\vec{x}\, d\vec{y} \left[ \sum_{\alpha}\sum_{\gamma} \psi(\alpha)\psi(\gamma)\, \rho^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \right] \\ &+ \frac{\beta}{N(s-1)} \int d\vec{x} \sum_{\alpha} \psi^2(\alpha)\, \rho^{(1)}(\vec{x},\alpha) \end{aligned} \tag{4.14}$$

let us now relate this expression to the percolation picture, *i. e.*, to the limit $s \to 1$, when $\chi \to \beta S$ for densities $\rho < \rho_c$. For this range of densities, the symmetry of the system is completely unbroken and $\rho^{(1)}(\vec{x},\alpha)$ is independent of $\alpha$. From the normalization Eq. (4.2), it follows that

$$\int d\vec{x}\, \rho^{(1)}(\vec{x},\alpha) = \frac{1}{s} \int d\vec{x} \sum_{\alpha} \rho^{(1)}(\vec{x},\alpha) = N \tag{4.15}$$

Now $\sum_\alpha \psi^2(\alpha) = (s-1)^2 + (s-1)(-1)^2$, so that

$$\lim_{s\to 1} \frac{1}{s-1} \sum_{\alpha} \psi^2(\alpha) = 1 \tag{4.16}$$

and therefore

$$\frac{\beta}{N(s-1)} \int d\vec{x} \sum_{\alpha} \psi^2(\alpha)\, \rho^{(1)}(\vec{x},\alpha) = \beta \tag{4.17}$$

Hence, when $s \to 1$,

$$\frac{\chi}{\beta} \to S = 1 + \lim_{s\to 1} \frac{1}{N(s-1)} \int d\vec{x}\, d\vec{y} \left[ \sum_{\alpha} \sum_{\gamma} \psi(\alpha)\psi(\gamma)\rho^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \right] \tag{4.18}$$

Let us now recalculate this quantity by using the general connection between averages in the Potts fluid and in the percolation model, Eq. (2.23). In particular,we have

$$\left\langle \frac{\beta}{N(s-1)} \sum_{i\neq j} \psi(\lambda_i)\psi(\lambda_j) \right\rangle_s = \frac{\beta}{N(s-1)} \sum_{i\neq j} \left\langle \sum_{\{\lambda_m:cl.\}} \psi(\lambda_i)\psi(\lambda_j) \right\rangle_p \tag{4.19}$$

where we have already set $h = 0$, which is allowed since in the range $\rho < \rho_c$, the symmetry is unbroken anyway. Let us now calculate the average on the r.h.s separately when $\lambda_i$ and $\lambda_j$ belong to the same cluster and when they do not. To this end, define a function $\Omega(i,j)$ as

$$\Omega(i,j) = \begin{cases} 1 & \text{if} \quad i,j \quad \text{belong to the same cluster} \\ 0 & \text{otherwise} \end{cases} \tag{4.20}$$

Then, from Eq. (2.21),

$$\begin{aligned} &\left\langle \sum_{\{\lambda_m:cl.\}} \psi(\lambda_i)\psi(\lambda_j) \right\rangle_p \\ &= \frac{1}{N!Z_p} \int d1 \cdots dN \sum_{\left\{ \substack{\text{conn.} \\ \text{states}} \right\}} P(\text{conn.}) \sum_{\{\lambda_m:cl.\}} \psi(\lambda_i)\psi(\lambda_j)\Omega(i,j) \\ &+ \frac{1}{N!Z_p} \int d1 \cdots dN \sum_{\left\{ \substack{\text{conn.} \\ \text{states}} \right\}} P(\text{conn.}) \sum_{\{\lambda_m:cl.\}} \psi(\lambda_i)\psi(\lambda_j)\,[1-\Omega(i,j)] \end{aligned} \tag{4.21}$$

The first sum contributes only if $\lambda_i, \lambda_j$ belong to the same cluster, while the second contributes only if they belong to separate clusters. Because of the geometrical mapping, $\psi(\lambda_i) = \psi(\lambda_j)$ in the first sum. Also, in the sum over $\{\lambda_m : cl\}$, every cluster other than the one containing $\lambda_i$ and $\lambda_j$ contributes a factor $s$, the number of possible spin assignments. The cluster containing $\lambda_i$ and $\lambda_j$ , on the other hand, contributes a factor $(s-1)^2$ if $\lambda_i = \lambda_j = 1$ and $(-1)^2$ for the $(s-1)$ other possible choices for $\lambda_i = \lambda_j$. Therefore,

$$\sum_{\{\lambda_m : cl.\}} \psi(\lambda_i)\psi(\lambda_j)\Omega(i,j) = s^{N_c-1}\left[(s-1)^2 + (s-1)(-1)^2\right]\Omega(i,j) \quad (4.22)$$

where $N_c$ is the total number of cluster in the configuration. Hence,

$$\begin{aligned} & \frac{\beta}{Z_p N(s-1)N!}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{conn.}) \sum_{\{\lambda_m : cl.\}} \psi(\lambda_i)\psi(\lambda_j)\Omega(i,j) \\ &= \frac{\beta}{N! Z_p N}\int d1\cdots dN \sum_{\left\{\substack{\text{conn.}\\ \text{states}}\right\}} P(\text{conn.}) s^{N_c-1}(s-1+1)\Omega(i,j) \\ &= \frac{\beta}{N}\left\langle s^{N_c}\Omega(\lambda_i,\lambda_j)\right\rangle_p \end{aligned} \quad (4.23)$$

The second sum in the r.h.s of Eq. (4.21) contributes only if $\lambda_i, \lambda_j$ belong to different clusters. The cluster containing $\lambda_i$ contributes a factor $(s-1)$ if $\lambda_i = 1$, and a factor $(-1)$ in all the other $(s-1)$ cases. The same holds for the cluster containing $\lambda_j$. The $N_c - 2$ remaining clusters contribute each a factor $s$. Hence,

$$\begin{aligned} & \sum_{\{\lambda_m : cl.\}} \psi(\lambda_i)\psi(\lambda_j)\left[1-\Omega(i,j)\right] \\ &= s^{N_c-2}\left[(s-1)+(s-1)(-1)\right]^2\left[1-\Omega(i,j)\right] = 0 \end{aligned} \quad (4.24)$$

We can now substitute the results Eqs. (4.23) and (4.24) into Eq. (4.10), then take again the limit $s \to 1$. Repeating the steps leading to Eq. (4.18), we end up this time with

$$\frac{\chi}{\beta} \to S = 1 + \frac{1}{N}\int d\vec{x}\, d\vec{y} \left\langle \sum_{i\neq j} \Omega(i,j)\delta(\vec{r}_i - \vec{x})\delta(\vec{r}_j - \vec{y}) \right\rangle_p \quad (4.25)$$

We define now the function

$$g^{\dagger}(\vec{x},\vec{y}) \equiv \frac{1}{\rho(\vec{x})\rho(\vec{y})}\left\langle \sum_{i\neq j} \Omega(i,j)\delta(\vec{r}_i - \vec{x})\delta(\vec{r}_j - \vec{y}) \right\rangle_p \quad (4.26)$$

to be the *pair connectedness* function [$\rho(\vec{x})$ is the density at position $\vec{x}$]. From the definition of $\Omega(i,j)$, the meaning of $g^\dagger$ is

$$\rho(\vec{x})\rho(\vec{y})\, g^\dagger(\vec{x},\vec{y})\, d\vec{x}d\vec{y} \quad = \quad \text{Probability of finding two particles in regions } d\vec{x} \text{ and } d\vec{y} \text{ around the positions } \vec{x} \text{ and } \vec{y}\text{, such that they both belong to the same cluster.} \tag{4.27}$$

which shows the pair-connectedness to be a generalization of the corresponding function in lattice percolation [16]. Hence,

$$S = 1 + \frac{1}{N}\int d\vec{x}\, d\vec{y}\ \rho(\vec{x})\rho(\vec{y})\, g^\dagger(\vec{x},\vec{y}) \tag{4.28}$$

Usually, the system is translationally invariant, so that $g^\dagger(\vec{x},\vec{y}) = g^\dagger(\vec{x}-\vec{y})$ and $\rho(\vec{x}) = \rho(\vec{y}) = \rho$. Then

$$S = 1 + \frac{V}{N}\rho^2 \int d\vec{r}\, g^\dagger(\vec{r}) = 1 + \rho \int d\vec{r}\, g^\dagger(\vec{r}) \tag{4.29}$$

Comparing Eq. (4.28) with Eq. (4.18), we finally obtain the important relationship

$$g^\dagger(\vec{x},\vec{y}) = \lim_{s\to 1} \frac{1}{(s-1)\rho^{(1)}(\vec{x})\,\rho^{(1)}(\vec{y})} \sum_\alpha \sum_\gamma \psi(\alpha)\psi(\gamma)\rho^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \tag{4.30}$$

Let us now introduce the spin pair-correlation function, defined as

$$g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \equiv \frac{1}{\rho^{(1)}(\vec{x})\,\rho^{(1)}(\vec{y})}\rho^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \tag{4.31}$$

which tends to 1 when $|\vec{x}-\vec{y}| \to \infty$. We can now rewrite Eq. (4.30) as

$$g^\dagger(\vec{x},\vec{y}) = \lim_{s\to 1} \frac{1}{s-1} \sum_\alpha \sum_\gamma \psi(\alpha)\psi(\gamma)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \tag{4.32}$$

or

$$\begin{aligned} g^\dagger(\vec{x},\vec{y}) \quad &= \quad \lim_{s\to 1} \frac{1}{s-1} \sum_\alpha \psi^2(\alpha) g_s^{(2)}(\vec{x},\alpha;\vec{y},\alpha) \\ &+ \quad \lim_{s\to 1} \frac{1}{s-1} \sum_{\alpha\neq\gamma} \psi(\alpha)\psi(\gamma) g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \end{aligned} \tag{4.33}$$

We now have

$$\sum_{\alpha} \psi^2(\alpha) g_s^{(2)}(\vec{x},\alpha;\vec{y},\alpha) = (s-1)^2 g_s^{(2)}(\vec{x},1;\vec{y},1) + (s-1)(-1)^2 g_s^{(2)}(\vec{x},\sigma;\vec{y},\sigma) \tag{4.34}$$

where $\sigma$ is any value of the spin different from 1. As a result,

$$\lim_{s\to 1} \frac{1}{s-1} \sum_{\alpha} \psi^2(\alpha)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},\alpha) = \lim_{s\to 1} g_s^{(2)}(\vec{x},\sigma;\vec{y},\sigma) \tag{4.35}$$

where $\sigma \neq 1$.

Similarly,

$$\begin{aligned}
\sum_{\alpha\neq\gamma} \psi(\alpha)\psi(\gamma)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) &= (s-1) \sum_{\gamma\neq 1} \psi(\gamma)\, g_s^{(2)}(\vec{x},1;\vec{y},\gamma) \\
&+ (s-1) \sum_{\alpha\neq 1} \psi(\alpha)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},1) \\
&- \sum_{\alpha\neq 1} \sum_{\substack{\gamma\neq\alpha \\ \gamma\neq 1}} \psi(\alpha)\psi(\gamma)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) \\
&= (s-1)^2 \left[ g_s^{(2)}(\vec{x},1;\vec{y},\sigma) + g_s^{(2)}(\vec{x},\sigma;\vec{y},1) \right] \\
&+ (s-1)(s-2)\, g_s^{(2)}(\vec{x},\sigma;\vec{y},\eta)
\end{aligned} \tag{4.36}$$

where $\sigma \neq \eta$ are any values of the spin which are both different from 1. As a result,

$$\lim_{s\to 1} \frac{1}{s-1} \sum_{\alpha\neq\gamma} \psi(\alpha)\psi(\gamma)\, g_s^{(2)}(\vec{x},\alpha;\vec{y},\gamma) = -\lim_{s\to 1} g_s^{(2)}(\vec{x},\sigma;\vec{y},\eta) \tag{4.37}$$

Substituting Eqs. (4.35) and (4.37) into Eq. (4.33), we have, finally, that

$$g^{\dagger}(\vec{x},\vec{y}) = \lim_{s\to 1} \left[ g_s^{(2)}(\vec{x},\sigma;\vec{y},\sigma) - g_s^{(2)}(\vec{x},\sigma;\vec{y},\eta) \right] \qquad (\rho < \rho_c) \tag{4.38}$$

where $\sigma, \eta \neq 1$ and $\sigma \neq \eta$.

This last equation is easily understood in terms of the geometrical mapping. If two particles $\vec{x}$ and $\vec{y}$ belong to the same cluster, they must have the same spin, say a spin $\sigma$. Hence $g^{\dagger}(\vec{x},\vec{y})$ must be contained in $g_s^{(2)}(\vec{x},\sigma;\vec{y},\sigma)$. However, $g_s^{(2)}(\vec{x},\sigma;\vec{y},\sigma)$ also includes the case where the two particles have the same spin but belong to different clusters. This happens if the two clusters have been assigned, by chance, the same overall spin. However, since such spin assignment is random, the probability of the two particles having the spins $\sigma$ and $\sigma$ (identical) is exactly the same as their having spins $\sigma$ and $\eta$, where now $\sigma \neq \eta$ (note that such an assignment automatically necessitates that the particles belong to different clusters). Hence $g_s^{(2)}(\vec{x}, \sigma; \vec{y}, \sigma)$ exceeds $g^{\dagger}(\vec{x}, \vec{y})$ by precisely $g_s^{(2)}(\vec{x}, \sigma; \vec{y}, \eta)$. This is the meaning of Eq. (4.38). It allows us to calculate the pair-connectedness by working out the spin pair-correlations and then taking the limit $s \to 1$. This completes the relation between the percolative quantities and those of the Potts fluid.

# 5 Conclusion

This paper has focused on the formal basis of continuum percolation theory. It has provided a non-perturbative definition of the fundamental quantities of the theory as well as showing formally how the binding criterion $p(\vec{r})$ and the interaction $v(\vec{r})$ enter them. We have seen that the quantities of interest in continuum percolation can be obtained from the $s \to 1$ limit of the Potts fluid. Specifically, the magnetization and the susceptibility become in this limit the percolation probability and the mean cluster size, respectively, while the pair-connectedness is, in this limit, the difference between two Potts pair-correlation functions.

The advantage of this mapping is that the Potts fluid has a Hamiltonian formulation. This is the key to applying the techniques of equilibrium statistical mechanics and phase transitions to the problem of continuum percolation, a task which will be undertaken in future papers in this series. The line of attack is always to perform all calculations or theoretical derivations within the Potts fluid model, then to take the limit $s \to 1$ and thus obtain the corresponding values or expressions in the percolation system.

The first such technique that one would think to apply to any problem of phase transition is mean field theory. The Hamiltonian formulation of the Potts fluid allows a mean field approximation to be defined, while it would be far from obvious how to do this directly for the continuum percolation system. Mean field theory turns out to be non-trivial to derive because of the continuum nature of the system and the presence of interactions. It is the subject of the next paper.

# References


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