Percolation Theory

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Aim

The aim of the percolation theory course is to provide a challenging and stimulating introduction to a selection of topics within modern theoretical condensed matter physics.

Percolation theory is the simplest model displaying a phase transition. The analytic solutions to 1d and mean-field percolation are presented. While percolation cannot be solved exactly for intermediate dimensions, the model enables the reader to become familiar with important concepts such as fractals, scaling, and renormalisation group theory in a very intuitive way.

The text is accompanied by exercises with solutions and visual interactive simulations for the percolation theory model to allow the readers to experience the behaviour, in the spirit "seeing is believing". The animations can be downloaded via the URL http://www.cmth.ph.ic.ac.uk/kim/cmth/

I greatly appriciate the suggestions and comments provided by Nicholas Moloney and Ole Peters without whom, the text would have been incomprehensible and flooded with mistakes. However, if you still are able to find **any** misprints, misspellings and mistakes in the notes, I would be very grateful if you would report those to k.christensen@ic.ac.uk.

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1.1 Introduction

Percolation theory is the simplest not exactly solved model displaying a phase transition. Often, the insight into the percolation theory problem facilitates the understanding of many other physical systems. Moreover, the concept of fractals, which is intimately related to the percolation theory problem, is of general interest as it pops up more or less everywhere in Nature. The knowledge of percolation, fractals, and scaling are of immense importance theoretically in such diverse fields as biology, physics, and geophysics and also of practical importance in e.g. oil recovery. We will begin gently by developing a basic understanding of percolation theory, providing a natural introduction to the concept of scaling and renormalisation group theory.

1.2 Preliminaries

Let P(A) denote the probability for an event A and $P(A_1 \cap A_2)$ the joint probability for event A_1 and A_2 .

Definition 1 Two events A_1 and A_2 are independent $\Leftrightarrow P(A_1 \cap A_2) = P(A_1)P(A_2)$.

Definition 2 More generally, we define $n \geq 3$ events A_1, A_2, \ldots, A_n to be mutually independent if $P(A_1 \cap A_2 \cap \cdots \cap A_n) = P(A_1)P(A_2) \cdots P(A_n)$ and if any subcollection containing at least two but fewer than n events are mutually independent.

Let each site in a lattice be occupied at random with probability p, that is, each site is occupied (with probability p) or empty (with probability 1-p) independent of the status (empty or occupied) of any of the other sites in the lattice. We call p the occupation probability or the concentration.

Definition 3 A cluster is a group of nearest neighbouring occupied sites.

Percolation theory deals with the numbers and properties of the clusters formed when sites are occupied with probability p, see Fig. (1.1).

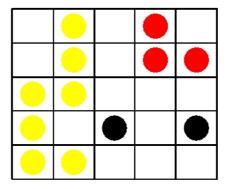


Figure 1.1: Percolation in 2d square lattice of linear size L = 5. Sites are occupied with probability p. In the lattice above, we have one cluster of size 7, a cluster of size 3 and two clusters of size 1 (isolated sites).

Definition 4 The cluster number $n_s(p)$ denotes the number of s-clusters per lattice site.

The (average) number of clusters of size s in a hypercubic lattice of linear size L is $L^d n_s(p)$, d being the dimensionality of the lattice. Defining the cluster number per lattice site as opposed to the total number of s-clusters in the lattice ensures that the quantity will be independent of the lattice size L.

For finite lattices $L < \infty$, it is intuitively clear, that if the occupation probability p is small, there is only a very tiny chance of having a cluster percolating between two opposite boundaries (i.e., in 2d, from top-to-bottom or from left-to-right). For p close to 1, we almost certainly will have a cluster percolating through the system. In Fig. 1.2, sites in 2d square lattices are occupied at random with increasing occupation probability p. The occupied sites are shown in gray while the sites belonging to the largest cluster are shown in black. Unoccupied sites are white. Note that for $p \approx 0.59$, a percolating cluster appears for the first time.

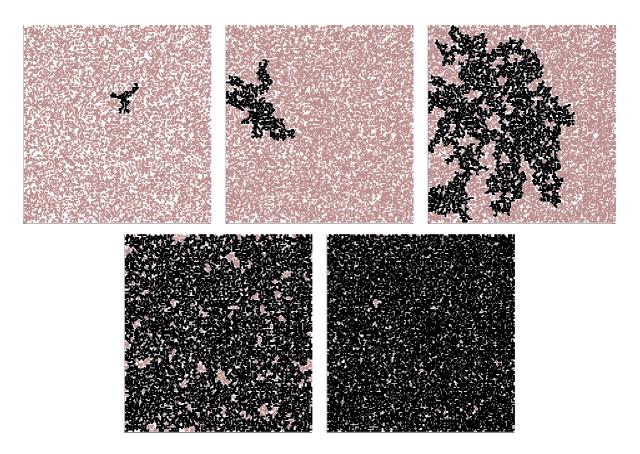


Figure 1.2: Percolation in 2d square lattices with system size $L \times L = 150 \times 150$. Occupation probability p = 0.45, 0.55, 0.59, 0.65, and 0.75, respectively. Notice, that the largest cluster *percolates* through the lattice from top to bottom in this example when $p \ge 0.59$.

Definition 5 The percolation threshold p_c is the concentration (occupation probability) p at which an infinite cluster appears for the first time in an infinite lattice.

Note, that p_c is defined with respect to an infinite lattice, that is, in the limit of $L \to \infty$. Table (1.1) lists the percolation threshold in various lattices and dimensions.

Exercise 1 Why is p_c not well defined in a finite lattice?

1.3 Percolation in 1d

We will consider the percolation problem in 1d where it can be solved analytically. Many of the characteristic features encountered in higher dimensions are present in 1d as well, if we know

Lattice	# nn	Site percolation	Bond percolation
1d	2	1	1
2d Honeycomb	3	0.6962	$1 - 2\sin(\pi/18) \approx 0.65271$
2d Square	4	0.592746	1/2
2d Triangular	6	1/2	$2\sin(\pi/18) \approx 0.34729$
3d Diamond	4	0.43	0.388
3d Simple cubic	6	0.3116	0.2488
3d BCC	8	0.246	0.1803
3d FCC	12	0.198	0.119
4d Hypercubic	8	0.197	0.1601
5d Hypercubic	10	0.141	0.1182
6d Hypercubic	12	0.107	0.0942
7d Hypercubic	14	0.089	0.0787
Bethe lattice	Z	1/(z-1)	1/(z-1)

Table 1.1: The percolation threshold for the site percolation problem is given in column 3 for various lattices in various dimensions. Column 2 lists the number of nearest-neighbours (nn), also known as the coordination number. Within a given dimension, the percolation threshold decrease with increasing number of nearest-neighbours. The site percolation problem has a counterpart called the bond percolation problem: In a lattice, each bond between neighbouring lattice sites can be occupied (open) with probability p and empty (closed) with probability p. A cluster is a group of connected occupied (open) bonds. NB: In all cases, a cluster is defined as a group of nearest neighbouring occupied sites (bonds). Note that the percolation threshold for the site-percolation on high-dimensional hypercubic lattices, where loops become irrelevant, approaches that of the Bethe lattice 1/(z-1), if we substitute the coordination number z with 2d.

where and how to look. Thus the 1d case serves as a transparent window into the world of phase transitions, scaling, scaling relations, and renormalisation group theory.

Imagine a 1d lattice with an infinite number of sites of equal spacing arranged in a line. Each site has a probability p of being occupied, and consequently 1-p of being empty (not occupied). These are the only two states possible, see Fig. 1.3.



Figure 1.3: Percolation in a 1d lattice. Sites are occupied with probability p. The crosses are empty sites, the solid circles are occupied sites. In the part of the infinite 1d lattice shown above, there is one cluster of size 5, one cluster of size 2, and three clusters of size 1.

What is of interest to us now and in future discussions in higher dimensions is the occupation probability at which an infinite cluster is obtained for the first time. A percolating cluster in 1d spans from $-\infty$ to $+\infty$. Clearly, in 1d this can only be achieved if all sites are occupied, that is, the percolation threshold $p_c = 1$, as a single empty site would prevent a cluster to percolate.

A precise "mathematical" derivation of $p_c = 1$ in 1d goes as follows.

Definition 6 Let $\Pi(p,L)$ denote the probability that a lattice of linear size L percolates at concentration p.

Combining the two definitions (5) and (6), we have,

$$\lim_{L \to \infty} \Pi(p, L) = \begin{cases} 0 & \text{for } p < p_c \\ 1 & \text{for } p \ge p_c. \end{cases}$$

Consider a finite 1d lattice of size L where each site is occupied with probability p. As the events of occupying sites are independent, all sites are occupied with probability $\Pi(p, L) = p^L$, see Fig. (1.4), and

$$\lim_{L \to \infty} \Pi(p, L) = \lim_{L \to \infty} p^L = \begin{cases} 0 & \text{for } p < 1\\ 1 & \text{for } p = 1, \end{cases}$$

implying $p_c = 1$.

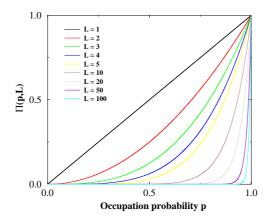


Figure 1.4: The probability of a 1d lattice of linear size L to percolation at occupation probability p. In the limit $L \to \infty$, $\Pi(p, L)$ converges to a discontinuous step function.

Let us consider the clusters formed in a 1d lattice. A cluster of size s is formed when s sites are occupied next to one another bounded by two empty sites, see Fig. 1.3. When $L \to \infty$, we can ignore the effects of the boundary sites of the lattice and the probability of an **arbitrary** site (occupied or not) being, say, the left hand side (LHS) of an s-cluster is

$$n_s(p) = (1-p)p^s(1-p) = (1-p)^2p^s.$$
 (1.1)

This expression is obtained from the assumption that the occupancy of each site is **independent** of the state of any other site. If this was not the case then it would be much more complicated. Note that, since all sites have equal probability of being occupied (or empty), the probability that an arbitrary site is part of an s-cluster is s times the probability of it being the LHS of the cluster.

We can re-write the cluster number Eq.(1.1) for 1d percolation as

$$n_{s}(p) = (1-p)^{2} p^{s}$$

$$= (1-p)^{2} \exp(\ln(p^{s}))$$

$$= (1-p)^{2} \exp(s \ln(p))$$

$$= (p_{c}-p)^{2} \exp(-\frac{s}{s_{\xi}})$$
(1.2)

with the definition of a cutoff cluster size or characteristic cluster size

$$s_{\xi} = \frac{-1}{\ln(p)} = \frac{-1}{\ln(p_c - (p_c - p))} \to \frac{1}{p_c - p} = (p_c - p)^{-1}$$
 for $p \to p_c$, (1.3)

where we, to obtain the limit, have used $p_c = 1$ and the Taylor expansion

$$\ln(1-x) = -x - \frac{1}{2}x^2 - \frac{1}{3}x^3 - \dots \approx -x$$

where the last approximation is valid for $x \to 0$, see Fig. 1.5.

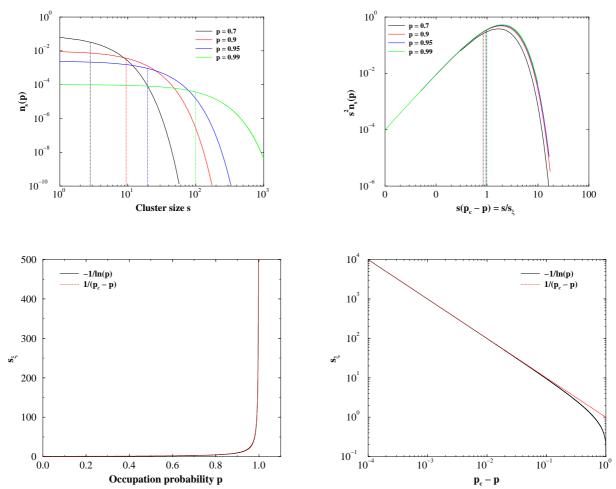


Figure 1.5: Percolation in 1d. (a) The cluster number distribution $n_s(p) = (p_c - p)^2 \exp(-\frac{s}{s_{\xi}})$ for various values of p approaching $p_c = 1$. The vertical lines indicate the cutoff cluster size $s_{\xi}(p)$. (b) By plotting $s^2 n_s(p)$ versus $s/s_{\xi} \approx s(p_c - p)$, all the data collapses onto a function $x^2 \exp(-x)$. (c) The characteristic cluster size $s_{\xi} = -\frac{1}{\ln(p)}$ diverges when $p \to p_c = 1$. (d) In the limit $p \to p_c = 1$, $s_{\xi} \propto (p_c - p)^{-1}$.

Exercise 2 Verify the Taylor expansion of $\ln(1-x)$ around x=0 given above.

Thus the cutoff cluster size s_{ξ} diverges for $p \to p_c$ as a power law in the distance from the critical occupation probability p_c , see Fig. 1.5. The divergence of the cutoff cluster size when $p \to p_c$ is also seen in higher dimensions where, however, another numerical exponent will describe the divergence. Thus it is natural to introduce a symbol for the exponent.

Definition 7 The critical exponent σ is defined by

$$s_{\xi} \propto |p_c - p|^{-\frac{1}{\sigma}} \qquad \text{for } p \to p_c.$$
 (1.4)

In 1d percolation theory, $\sigma = 1$ and $\log s_{\xi} = \text{constant} - \frac{1}{\sigma} \log |p_c - p|$, see Fig. 1.5.

Let us continue our journey into 1d percolation theory. For $p < p_c$ we can state that the probability that an arbitrary site belongs to **any** (finite) cluster is simply the probability p of it being occupied. Since the probability that an arbitrary sites belongs to an s-cluster is given by $sn_s(p)$, we arrive at

$$\sum_{s=1}^{\infty} s n_s(p) = p \qquad \text{for } p < p_c.$$
 (1.5)

Using the formula for summing a geometric series, we can satisfy those who prefer a rigorous mathematical proof:

$$\sum_{s=1}^{\infty} s n_s(p) = \sum_{s=1}^{\infty} s (1-p)^2 p^s$$

$$= (1-p)^2 \sum_{s=1}^{\infty} p \frac{d(p^s)}{dp}$$

$$= (1-p)^2 p \frac{d}{dp} \left(\sum_{s=1}^{\infty} p^s\right)$$

$$= (1-p)^2 p \frac{d}{dp} \left(\frac{p}{1-p}\right)$$

$$= p.$$

How large on average is a cluster or, equivalently, how large is a cluster on average to which an occupied site belongs? The probability that a site is occupied is p. The probability that an arbitrary site belongs to an s-cluster is $sn_s(p)$. Thus the probability w_s that the cluster to which an occupied sites belongs contains s sites is

$$w_s = \frac{sn_s(p)}{p} = \frac{sn_s(p)}{\sum_{s=1}^{\infty} sn_s(p)}.$$

Thus, the mean cluster size or average cluster size S(p) is given by

$$S(p) = \sum_{s=1}^{\infty} sw_s$$

$$= \sum_{s=1}^{\infty} \frac{s^2 n_s(p)}{\sum_{s=1}^{\infty} n_s(p)s}$$

$$= \frac{1}{p} (1-p)^2 \sum_{s=1}^{\infty} s^2 p^s$$

$$= \frac{1}{p} (1-p)^2 \left(p \frac{d}{dp}\right)^2 \left(\sum_{s=1}^{\infty} p^s\right),$$

where the operator

$$\left(p\frac{d}{dp}\right)^2 = \left(p\frac{d}{dp}\right)\left(p\frac{d}{dp}\right) \neq p^2\frac{d^2}{dp^2}.$$

Using the formula for summing a geometric series and the operator $p\frac{d}{dp}$ twice, we finally arrive at

$$S(p) = \frac{1+p}{1-p} = \frac{p_c + p}{p_c - p} \tag{1.6}$$

where the last equality follows because in 1d the critical occupation probability $p_c = 1$.

Exercise 3 Derive the result in Eq. (1.6) for the mean cluster size in 1d.

We thus see that the mean cluster size diverges for $p \to p_c^-$, where the minus sign signifies that we are approaching p_c from below, which is what we intuitively expect if considering an infinite lattice. It is not possible to approach p_c from above in 1d as $p_c = 1$. This is actually the main difference between 1d and higher dimensions, where, $p_c < 1$ and we can approach p_c from both below and above.

In order to investigate in detail how the mean cluster size diverges, when taking the limit $p \to p_c^-$, we note that the numerator in Eq.(1.6) approaches $2p_c$, so

$$S(p) = \frac{p_c + p}{p_c - p} \to \frac{2p_c}{p_c - p} \propto (p_c - p)^{-1}$$
 for $p \to p_c^-$. (1.7)

Thus in 1d, the mean cluster diverges like a power law in the quantity $(p_c - p)$ when $p \to p_c$, see Fig. 1.6. The same phenomenon will be encountered in higher dimensions.

Definition 8 The critical exponent γ is defined by

$$S(p) \propto |p_c - p|^{-\gamma} \qquad \text{for } p \to p_c.$$
 (1.8)

In 1d percolation theory, $\gamma = 1$.

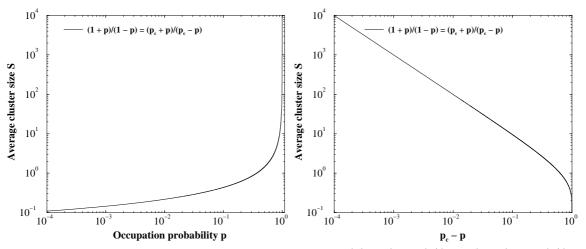


Figure 1.6: Percolation in 1d. The average cluster size $S(p) = (1+p)/(1-p) = (p_c+p)/(p_c-p)$ diverges when $p \to p_c = 1$. In the limit $p \to p_c = 1$, $S(p) \to 2/(p_c-p)$.

Definition 9 The correlation function or pair connectivity $g(\mathbf{r})$ is the probability that a site at position \mathbf{r} from an occupied site belongs to the same finite cluster.

Note this definition excludes the contribution from the infinite cluster. That need not worry us in 1d, where all clusters are finite if $p < p_c = 1$. Let $r = |\mathbf{r}|$. Clearly, $g(\mathbf{r} = \mathbf{0}) = 1$, since the site is occupied by definition. In 1d, for a site at position \mathbf{r} to be occupied and belong to the same (finite) cluster, this site and the (r-1) intermediate sites must be occupied, leaving

$$q(\mathbf{r}) = p^r$$

for all p, which can also be expressed in the form

$$g(\mathbf{r}) = \exp(\ln(p^r)) = \exp(r\ln(p)) = \exp\left(-\frac{r}{\xi}\right),\tag{1.9}$$

where

$$\xi = -\frac{1}{\ln(p)} = \frac{-1}{\ln(p_c - (p_c - p))} \to \frac{1}{(p_c - p)} = (p_c - p)^{-1}$$
 for $p \to p_c = 1$, (1.10)

where we use the expansion $\ln(1-x) \approx -x$ for small x. The quantity ξ is called the *correlation length* which diverges for $p \to p_c$. The same phenomenon will be encountered in higher dimensions. Note that in 1d we have $s_{\xi} = \xi$ which is why we haven't bothered displaying a figure for ξ , as it would be identical to Fig. 1.5. However, this identity will not be true in higher dimensions, where we will find $s_{\xi} \propto \xi^D$, where D is the fractal dimension, but more about this later.

Definition 10 The critical exponent ν is defined by

$$\xi \propto |p_c - p|^{-\nu}$$
 for $p \to p_c$. (1.11)

In 1d percolation theory, $\nu = 1$.

By summing over all possible lattice sites \mathbf{r} of the correlation function, the mean cluster size can be shown to be

$$\sum_{\mathbf{r}} g(\mathbf{r}) = S(p). \tag{1.12}$$

In 1d, this sum is straight forward identifying \mathbf{r} with $r = 0, \pm 1, \pm 2, \ldots$, see *Problem 2*, where you will also discover, that the sum rule is valid in all dimensions d.

The general pattern for the exact solutions of the 1d percolation problem is that certain quantities, such as the cutoff cluster size s_{ξ} , the mean cluster size S(p), and the correlation length ξ diverge at the percolation threshold. The divergence can be described by simple power laws of the distance from the critical occupation probability $|\Delta p| = |p_c - p|$, e.g. $\xi \propto (p_c - p)^{-1}$, at least asymptotically close to p_c where Δp is small. The same phenomena will be encountered in higher dimensions even though we cannot obtain exact analytic solutions.

1.4 Percolation in the Bethe Lattice

The percolation problem can be solved analytically in d=1 and $d=\infty$. The infinitely dimensional case is synonymous with the Bethe lattice, a special lattice where each site has z neighbouring sites, such that each *branch* gives rise to z-1 other branches, see Fig. 1.7.

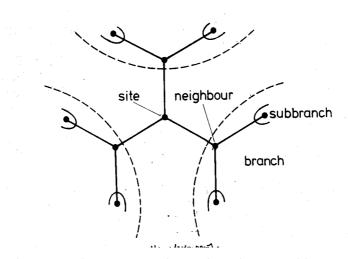


Figure 1.7: The Bethe lattice with z=3. Each site has three neighbours. Each branch contains z-1=2 subbranches.

The 1d case is effectively a Bethe lattice with z=2. Why does the Bethe lattice correspond to the spatial dimension $d=\infty$ you might rightly ask! Well, in a hypercubic lattice, (a) the number of surface sites relative to the total number of sites approaches a constant when $d\to\infty$ and (b) there are no closed loops when $d\to\infty$. The Bethe lattice has both these properties.

(a) Let g denote the generation, that is, the distance from a "centre site". Note, however, that in an infinite Bethe lattice, all sites are equivalent, so the notion of a "centre site" is not to be taken literally. In the figure above, the first "ring" of three sites belong to generation g = 1, the second "ring" of six sites belongs to the second generation and so on. The total number of sites in a Bethe lattice consisting of g generations is

Total no. sites =
$$1 + 3 \cdot (1 + 2 + \dots + 2^{g-1})$$

= $1 + 3 \cdot \frac{1 - 2^g}{1 - 2}$
= $3 \cdot 2^g - 2$.

while the number of surface sites is $3 \cdot 2^{g-1}$. Thus

$$\frac{\text{No. of surface sites}}{\text{Total no. of sites}} = \frac{3 \cdot 2^{g-1}}{3 \cdot 2^g - 2} \to \frac{1}{2} \qquad \text{ for } g \to \infty.$$

and the surface/volume tends to a constant.

Exercise 4 Show, that for a general Bethe lattice with coordination number z

$$\frac{No. \ of \ surface \ sites}{Total \ no. \ of \ sites} \rightarrow \frac{z-2}{z-1} \qquad for \ g \rightarrow \infty.$$

In a hypercubic lattice of linear size L, the surface is proportional to the volume only when $d \to \infty$: the surface in d dimensions is proportional to L^{d-1} while the volume is proportional to L^d leaving

Surface
$$\propto \text{Volume}^{\frac{d-1}{d}} = \text{Volume}^{1-\frac{1}{d}}$$

that is, the surface is proportional to the volume if $d \to \infty$.

(b) There are no closed loops in a Bethe lattice. Starting from the "centre site" going outwards, one will never return to the starting point. In a hypercubic lattice, the chance (probability) of having a loop approaches zero as the dimension $d \to \infty$: As an example, let us place four particles in a chain in a hypercubic lattice with dimension d. When the first particle has been placed, there are 2d nearest neighbour sites, where the second particle can be placed. However, for the third and fourth particle, there are only 2d - 1 possible sites, implying a total no. of different chains $2d \cdot (2d - 1)^2$. Calculating the number of ways to place four particles in a loop, we arrive at $2d \cdot (2d - 2) \cdot 1$, that is, the probability of having a four loop

$$\frac{\text{No. loops}}{\text{Total no. chains}} = \frac{2d \cdot (2d-2) \cdot 1}{2d \cdot (2d-1)^2} = \frac{(2d-2)}{(2d-1)^2} \to 0 \qquad \text{ for } d \to \infty.$$

For $d = \infty$, there is no chance of having a closed loop, which is intuitively clear, isn't it?

What is the critical occupation probability in a Bethe lattice, that is, at which occupation probability does an infinite cluster (path) appear for the first time in an infinite Bethe lattice? Starting from a "centre site" and going outwards, we encounter (z-1) new neighbours. Thus, on average, we have p(z-1) new occupied sites on which we can continue the path. The critical occupation probability is determined by the equation

$$p_c(z-1) = 1 \Leftrightarrow p_c = \frac{1}{z-1}.$$

Notice, that for z=2, the 1d percolation problem, we recover $p_c=1$. For z=3, e.g., $p_c=\frac{1}{2}$. Note that in a hypercubic lattice with $d\to\infty$ one would expect $p_c\to 1/(2d-1)$ in order to be able to continue walking along a path of occupied sites.

Definition 11 The strength of the infinite cluster P(p) is the probability that an arbitrary site belongs to the infinite cluster.

Exercise 5 Discuss why, obviously, P(p) = 0 for $p < p_c$ in an infinite lattice.

In order to calculate P(p) for $p > p_c$ in the Bethe lattice, we introduce the quantity Q as the probability that an arbitrary site is **NOT** connected to infinity through a fixed branch originating at this site. Restricting ourselves to the lattice with z = 3 and using basic probability theory, we have that the strength P(p) of the infinite network, that is, the probability that an arbitraryly selected site is connected to infinity by occupied sites is

$$P(p) = (\text{Prob. site is occupied}) \times (\text{Prob. at least ONE branch lead to infinity})$$

= $p(1-Q^3)$.

Next, we need to determine Q, the probability that a branch originating at that site does not lead to infinity. This depends on whether or not the neighbouring site is occupied. We find

$$Q = (\text{Prob. site is empty}) + (\text{Prob. site is occupied}) \times (\text{Prob. no subbranch leads to infinity})$$

= $(1-p) + pQ^2$.

We have relied on the fact that all sites in a Bethe lattice are equivalent, so Q is also the probability that a **sub**branch is not connected to infinity. The quadratic equation can easily be solved:

$$Q = \frac{1 \pm \sqrt{(2p-1)^2}}{2p} = \begin{cases} 1 \\ \frac{1-p}{p}. \end{cases}$$

Exercise 6 Show that, in a general Bethe lattice where each site has z neighbours (Problem 4),

$$Q = \begin{cases} 1 \\ 1 - \frac{2p(z-1)-2}{p(z-1)(z-2)}. \end{cases}$$

When $p < p_c$, there are no infinite clusters, by definition, so with probability 1 there is no connection to infinity. Thus Q = 1 is the *trivial solution* associated with P(p) = 0 for $p < p_c$. The non-trivial solution $Q = \frac{1-p}{p}$ is associated with $p > p_c$, leaving

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p \left(1 - \left(\frac{1-p}{p}\right)^3\right) & \text{for } p \ge p_c. \end{cases}$$

Using a Taylor expansion for P(p) around $p = p_c = \frac{1}{2}$, it can be shown that (see Problem 4)

$$P(p) \propto (p - p_c)$$
 for $p \to p_c^+$.

Definition 12 The critical exponent β is defined by

$$P(p) \propto (p - p_c)^{\beta}$$
 for $p \to p_c^+$. (1.13)

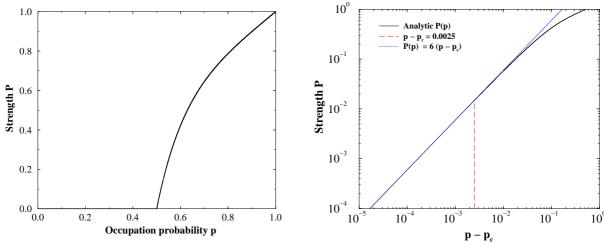


Figure 1.8: The strength P(p) of the infinite cluster in a Bethe lattice with z=3. When $p \to p_c^+$, the strength $P(p) \to 6(p-p_c)$ implying $\beta=1$ in a Bethe lattice.

In the Bethe lattice, $\beta = 1$, see Fig. 1.8.

The strength P(p) measures how large a fraction of the sites in the lattice belongs to the infinite cluster (in an infinite lattice) and is known as the *order parameter*. The phenomenon that the order parameter (strength) becomes non-zero for $p > p_c$ is known as a phase transition and $p = p_c$ is often called a critical point or critical occupation probability.

Exercise 7 What is the strength P(p) in the 1d percolation problem?

What is the mean cluster size S(p) to which an occupied site (e.g. the "centre site") belongs? Let T be the mean cluster size in one branch.

S(p) = average cluster size to which the origin belongs = (contribution from origin) + (contributions from the 3 branches) = 1 + 3T.

Thus, we have to determine T. Again, as all sites are equivalent in an infinite Bethe lattice, T will also denote the mean cluster size in the **sub**branch, so we can argue as follows: If the neighbour to the "centre site" is empty, probability (1-p), there is no contribution to T from this branch. If the neighbour to the "centre site" is occupied (probability p), it contributes its own mass (unity) to the cluster, and adds the mass T for each of its z-1=2 subbranches. Thus,

$$T = (1-p) \cdot 0 + p \cdot (1+2T) \Leftrightarrow T = \frac{p}{1-2p} \quad \text{for } p < p_c.$$

Therefore, the mean cluster size S(p) is given by

$$S(p) = 1 + 3T = \frac{1+p}{(1-2p)} = \frac{1+p}{2(\frac{1}{2}-p)} = \frac{1+p}{2(p_c-p)} = \Gamma_2(p_c-p)^{-1},$$
 (1.14)

where $\Gamma_2 = \frac{1+p}{2}$ is the amplitude, and the critical exponent $\gamma = 1$ in the Bethe lattice. This is the exact result for a mean cluster of size S(p) and we notice that it diverges for $p \to p_c$.

An occupied site either belongs to the infinite cluster or a finite cluster. Thus, the generalisation of Eq.(1.5) is valid for all p

$$P(p) + \sum_{s=1}^{\infty} s n_s(p) = p \qquad \forall p.$$
 (1.15)

The sum runs over all **finite** s and **excludes** the infinite cluster. Of course, Eq.(1.15) reduces to Eq.(1.5) for $p < p_c$ since the strength P(p) is identical zero in this range.

Exercise 8 Reflect upon the identity Eq.(1.15) for $p = p_c$. What is the sum $\sum_{s=1}^{\infty} sn_s(p_c)$? Is your answer also valid in d = 1?

Critical phenomena occur in a variety of systems. The Bethe lattice approximation for percolation theory is somewhat analogous to the mean-field approximation for magnetic systems dislaying a phase transition, or the Van der Waals equation for a fluid. In all cases, the order parameter becomes non-zero above (or below) the critical point. In a magnetic system, the order parameter is the spontaneous magnetisation per spin m, which is zero above the critical temperature (Curie temperature) T_c and non-zero for $T < T_c$ as the system enters an ordered state. We will see later, that $m \propto (T_c - T)^{\beta}$. In the case of a fluid, the order parameter is identified as the the difference between liquid and vapour density which becomes nonzero as $T < T_c$. The analogy between mean-field thermal critical phenomena and percolation is not complete since the critical exponent β for the order parameter is $\frac{1}{2}$ for thermal phase transitions and unity for percolation, but nevertheless, the qualitative similarities are clear.

In both the thermal phase transitions mentioned above and percolation, the order parameter goes to zero continuously as one approaches the critical point. Such phase transitions are called continuous phase transitions or *second-order* phase transitions. If instead the order parameter jumps to zero, one has a *first order* phase transition. Such transitions can occur in more complicated percolation theory situations, like "bootstrap percolation" where on a square lattice a site remains occupied only if three or four of its neighbours are still occupied [2].

1.5 Cluster Number Distribution

Unfortunately, it is not possible to obtain an exact form for the cluster number $n_s(p)$ in d > 1 or the Bethe lattice since, unlike in 1d, there are a very large number of different ways in which clusters can arrange themselves. Even for relatively small cluster numbers in 2d we run into difficulties. Exact enumeration of small cluster "animals" has been tabulated. In a 2d square lattice a computer has counted a total of 68,557,762,666,345,165,410,168,738 different cluster configurations with s = 46 [3]. Nevertheless, we are still able to account for the general scaling behaviours of certain quantities that characterise the clusters.

Definition 13 The perimeter or external boundary t of a cluster is the number of empty nearest neighbours of the cluster.

Using the concept of a perimeter, we are able write down the general expression for the cluster number $n_s(p)$ as

$$n_s(p) = \sum_{t} g_{s,t} p^s (1-p)^t, \tag{1.16}$$

where we have introduced $g_{s,t}$, the number of different lattice configurations with size s and perimeter t.

In 1d, all clusters have two perimeter sites and thus

$$g_{s,t} = \begin{cases} 1 & \text{for } t = 2\\ 0 & \text{otherwise} \end{cases}$$

implying $n_s(p) = p^s(1-p)^2$.

Exercise 9 Consider clusters of size s=3 in 2d on a square lattice. Verify, that $g_{s,t}$ is only non-zero for t=7 or t=8 and that $g_{s=3,t=7}=4$ and $g_{s=3,t=8}=2$, implying $n_{s=3}(p)=4p^3(1-p)^7+2p^3(1-p)^8$.

In a Bethe lattice, however, we can show that there is a unique perimeter for a given cluster size s.

Exercise 10 Show that in a Bethe lattice t = 2 + s(z - 2).

Now we apply this formula to our general result for cluster numbers (1.16) to get:

$$n_s(p) = \sum_{t} g_{s,t} p^s (1-p)^t = g_{s,2+s(z-2)} p^s (1-p)^{2+s(z-2)}.$$
(1.17)

For simplicity, from here on we shall work with the z=3 case rather than the general Bethe lattice. For z=3 we have $p_c=\frac{1}{2}$. As we have said, determining $g_{s,2+s}$ for large s is difficult, but we can avoid having to calculate $g_{s,2+s}$ by considering the ratio

$$\frac{n_s(p)}{n_s(p_c)} = \left[\frac{(1-p)}{(1-p_c)}\right]^2 \left[\left(\frac{p}{p_c}\right) \frac{(1-p)}{(1-p_c)}\right]^s \\
= \left[\frac{(1-p)}{(1-p_c)}\right]^2 \exp\left[s \ln\left(\frac{p}{p_c} \frac{(1-p)}{(1-p_c)}\right)\right].$$
(1.18)

In order to proceed, define the function

$$f(p) = \frac{p}{p_c} \frac{(1-p)}{(1-p_c)} = \frac{p}{\frac{1}{2}} \frac{(1-p)}{(1-\frac{1}{2})} = 4p - 4p^2$$
 for $z = 3$.

Exercise 11 Make a Taylor expansion of the function $f(p) = 4p - 4p^2$ around $p = \frac{1}{2} = p_c$ and verify $f(p) = 1 - 4(p - p_c)^2$.

Substituting the expression for f(p) given in Exercise 11, we find

$$\frac{n_s(p)}{n_s(p_c)} = \left[\frac{(1-p)}{(1-p_c)}\right]^2 \exp(-\frac{s}{s_{\xi}})$$
 (1.19)

with

$$s_{\xi} = \frac{-1}{\ln\left(1 - 4\left(p - \frac{1}{2}\right)^{2}\right)}$$

$$\propto \frac{1}{4}\left(p - \frac{1}{2}\right)^{-2} \quad \text{for } p \to \frac{1}{2}$$

$$\propto |p - p_{c}|^{-\frac{1}{\sigma}}. \tag{1.20}$$

In the Bethe lattice, $\sigma = \frac{1}{2}$.

We now have a very simple exponential decay for the ratio of cluster numbers. This is to say that large clusters with $s \gg s_{\xi}$ are very rare indeed. This explains why s_{ξ} is known as the cutoff cluster size. In order to investigate the cluster number distribution in more detail, we have to consider the term $n_s(p_c)$ appearing in the denominator.

From the analysis on the average cluster size, we know that,

$$S(p) = \sum_{s=1}^{\infty} \frac{s^2 n_s(p)}{\sum_{s=1}^{\infty} s n_s(p)} \to \infty \qquad \text{for } p \to p_c.$$
 (1.21)

However, the denominator remains finite at $p = p_c$ (why?) so the numerator must diverge for $p = p_c$, that is,

$$\sum_{s=1}^{\infty} s^2 n_s(p_c) = \infty.$$

Generally, we have that

$$\sum_{s=1}^{\infty} s^a = \begin{cases} \text{convergent for } a < -1\\ \text{divergent for } a \ge -1. \end{cases}$$

Thus a power-law decay

$$n_s(p_c) \propto s^{-\tau} \Rightarrow \sum_{s=1}^{\infty} s^2 n_s(p_c) = \sum_{s=1}^{\infty} s^{2-\tau}$$

would imply a divergence of the average cluster size if the critical exponent $\tau \leq 3$.

However, see Eq.(1.15) and problem (8), we also need $p_c = \sum_{s=1}^{\infty} s n_s(p_c) \propto \sum_{s=1}^{\infty} s^{1-\tau} < \infty$ implying that $\tau > 2$. Therefore, we arrive at a general form for the cluster number distribution in the Bethe lattice:

$$n_s(p) \propto s^{-\tau} \exp(-\frac{s}{s_{\xi}}), \text{ for } s \gg 1$$
 (1.22)

with

$$s_{\xi} \propto |p_c - p|^{-\frac{1}{\sigma}} \quad \text{for } p \to p_c,$$
 (1.23)

where $\sigma = \frac{1}{2}$ and $2 < \tau \le 3$.

Actually, we can determine τ as it is not independent of the critical exponents γ and σ determined previously. Let us evaluate the average cluster size S(p) assuming Eq.(1.22) is valid for all s. Neglecting the denominator which for $p \to p_c$ will approach p_c and thus be a constant we find

$$S(p) \propto \sum_{s=1}^{\infty} s^{2} n_{s}(p)$$

$$\propto \sum_{s=1}^{\infty} s^{2-\tau} \exp(-\frac{s}{s_{\xi}})$$

$$\approx \int_{1}^{\infty} s^{2-\tau} \exp(-\frac{s}{s_{\xi}}) ds$$

$$= \int_{1/s_{\xi}}^{\infty} (zs_{\xi})^{2-\tau} \exp(-z) s_{\xi} dz \quad \text{with } z = s/s_{\xi}$$

$$= s_{\xi}^{3-\tau} \int_{1/s_{\xi}}^{\infty} z^{2-\tau} \exp(-z) dz$$

$$= s_{\xi}^{3-\tau} \int_{0}^{\infty} z^{2-\tau} \exp(-z) dz \quad \text{for } p \to p_{c} \text{ where } s_{\xi} \to \infty$$

$$= s_{\xi}^{3-\tau} \Gamma(3-\tau) \qquad (1.24)$$

where Γ is the Gamma function

$$\Gamma(x) = \int_0^\infty z^{x-1} \exp(-z) \ dz.$$

Exercise 12 Show that the Gamma function Γ defined by the integral above satisfies the recursion relation $\Gamma(x+1) = x\Gamma(x)$ and deduce that $\Gamma(x+1) = x!$ for $x = 0, 1, 2, \ldots$ where 0! = 1.

Using $s_{\xi} \propto (p - p_c)^{-2}$, we see that

$$S(p) \propto (p - p_c)^{2\tau - 6} \propto (p - p_c)^{-1},$$
 (1.25)

where we have used Eq.(1.14). Thus we must require that

$$2\tau - 6 = -1 \Leftrightarrow \tau = \frac{5}{2}.\tag{1.26}$$

In summary, for the Bethe lattice

$$n_s(p) \propto s^{-\frac{5}{2}} \exp(-\frac{s}{s_{\xi}}) \qquad s \gg 1$$

 $s_{\xi} \propto |p - p_c|^{-2} \quad \text{for } p \to p_c.$

The above procedure is a general way of deriving a relationship between critical exponents, as we shall see shortly.

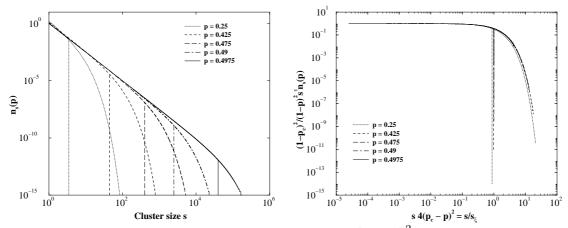


Figure 1.9: (a) The cluster number distribution $n_s(p) = \left[\frac{(1-p)}{(1-p_c)}\right]^2 s^{-\tau} \exp(-\frac{s}{s_{\xi}})$, see Eq.(1.19) for different values of p approaching $p_c = 1/(z-1) = 1/2$. The vertical lines indicate the cutoff cluster size $s_{\xi}(p)$ for the various p values. The cluster number distribution is well approximated by a power law for $s \ll s_{\xi}$ while is decays rapidly for $s \gg s_{\xi}$. (b) By plotting $\left[\frac{(1-p_c)}{(1-p)}\right]^2 s^{\tau} n_s(p)$ versus $s/s_{\xi} \approx s \cdot 4(p_c-p)^2$, all the data collapses onto the scaling function e^{-x} .

Now, we postulate a scaling ansatz (form) valid for all p and large s

Ansatz 1

$$n_s(p) \propto s^{-\tau} \exp(-\frac{s}{s_{\xi}}), \qquad s \gg 1,$$

 $s_{\xi} \propto |p - p_c|^{-\frac{1}{\sigma}} \qquad p \to p_c,$ (1.27)

or equivalently

$$n_s(p) \propto s^{-\tau} \exp(-s|p - p_c|^{\frac{1}{\sigma}})$$
 $s \gg 1$ and $p \to p_c$. (1.28)

Note the role of s_{ξ} as a cutoff cluster size, where $n_s(p)$ is characterised by

$$n_s(p) \propto \begin{cases} s^{-\tau} & \text{for } s \ll s_{\xi} \\ \text{decays rapidly} & \text{for } s \gg s_{\xi}, \end{cases}$$
 (1.29)

representing the crossover from a behaviour of "critical clusters" (power-law distributed) to that of non-critical clusters. Note also that $n_s(p_c) = s^{-\tau}$ as $s_{\xi} = \infty$ at $p = p_c$.

We can, however, immediately identify two problems (a third problem will surface shortly) with the scaling ansatz 1.

(1) The scaling ansatz 1 fails to describe the 1d case. We found previously that

$$n_s(p) = (1-p)^2 \exp(-\frac{s}{s_{\xi}}) = (p_c - p)^2 \exp(-\frac{s}{s_{\xi}}),$$

which is not a special case of our ansatz 1 since, instead of a power of s, we have $(p_c - p)^2$ in front of the exponential. You might be very tempted to say that $\tau = 0$, but that does actually not solve the problem, as we shall see below.

(2) For fixed s

$$n_s(p) = \sum_{t=1}^{\infty} g_{s,t} p^s (1-p)^t$$
 (1.30)

is a polynomial in p with a finite number of terms. Thus all derivatives of $n_s(p)$ with respect to p will remain finite for all p. However, using the scaling ansatz 1 for $p > p_c$ $n_s(p) = As^{-\tau} \exp(-s(p-p_c)^{\frac{1}{\sigma}})$ we find, keeping s constant

$$\frac{dn_s(p)}{dp} = As^{-\tau} \exp(-s(p - p_c)^{\frac{1}{\sigma}}) \frac{1}{\sigma} (p - p_c)^{\frac{1}{\sigma} - 1}$$
(1.31)

and by differentiating once more

$$\frac{d^2 n_s(p)}{dp^2} = A s^{-\tau} \left[\exp(-s(p - p_c)^{\frac{1}{\sigma}}) \left(\frac{1}{\sigma} (p - p_c)^{\frac{1}{\sigma} - 1} \right)^2 + \exp(-s(p - p_c)^{\frac{1}{\sigma}}) \frac{1}{\sigma} \left(\frac{1}{\sigma} - 1 \right) (p - p_c)^{\frac{1}{\sigma} - 2} \right].$$

In 2d, e.g., $\sigma = 0.4 \Leftrightarrow \frac{1}{\sigma} - 2 = 0.5$, so both the first and second derivative of $n_s(p)$ w.r.t. p remain finite as $p \to p_c$. The third derivative of $n_s(p)$, however, will contain a term with the factor $(p - p_c)^{\frac{1}{\sigma} - 3}$ which will diverge as $p \to p_c$ contrary to the derivatives of Eq.(1.30).

We shall later resolve these two problems, so there is no need for you to worry too much at the moment

Let us return to the question of deriving scaling relations assuming the scaling ansatz above for the cluster number distribution. Following the previous calculation of the average cluster size S(p)and noting that the Gamma function is just a number, we find

$$S(p) \propto s_{\xi}^{3-\tau} \propto |p - p_c|^{\frac{\tau - 3}{\sigma}}, \text{ for } p \to p_c,$$
 (1.32)

as

$$s_{\xi} \propto |p - p_c|^{-\frac{1}{\sigma}} \quad \text{for } p \to p_c.$$
 (1.33)

However, by definition

$$S(p) \propto |p - p_c|^{-\gamma} \quad \text{for } p \to p_c,$$
 (1.34)

implying the scaling relation

$$\gamma = \frac{3 - \tau}{\sigma}.\tag{1.35}$$

We notice again that to ensure the divergence of S(p) for $p \to p_c$ we must have $\tau < 3$ in order to leave $\gamma > 0$. Also, we recover problem (1) mentioned above because in 1d percolation theory $\gamma = 1$ and $\sigma = 1$ implying $\tau = 2$. However, there is no $s^{-\tau}$ term (yet!) in our expression for the 1d cluster number distribution $n_s(p)$ and obviously the suggested "solution" of assuming $\tau = 0$ is not valid either.

Now we focus our attention on the percolation strength P(p), starting from Eq.(1.15):

$$P(p) = p - \sum_{s=1}^{\infty} s n_s(p)$$

$$= p_c - \sum_{s=1}^{\infty} s n_s(p) + (p - p_c)$$

$$= \sum_{s=1}^{\infty} s n_s(p_c) - \sum_{s=1}^{\infty} s n_s(p) + \mathcal{O}(p - p_c) \quad (\mathcal{O}(p - p_c) = \text{term of order}(p - p_c))$$

$$= \sum_{s=1}^{\infty} s^{1-\tau} - \sum_{s=1}^{\infty} s^{1-\tau} \exp(-\frac{s}{s_{\xi}}) + \mathcal{O}(p - p_c) \quad \text{using the scaling ansatz 1}$$

$$\propto \sum_{s=1}^{\infty} s^{1-\tau} \left\{ 1 - \exp(-\frac{s}{s_{\xi}}) \right\} + \mathcal{O}(p - p_c).$$

$$\propto \sum_{s=1}^{\infty} s^{1-\tau} \left\{ 1 - \exp(-\frac{s}{s_{\xi}}) \right\} \Delta s, \tag{1.36}$$

where we have dropped the term of order $(p-p_c)$ and introduced $\Delta s=1$. When $p\to p_c$, the cutoff cluster size $s_\xi\to\infty$. Thus the term $\{1-\exp(-\frac{s}{s_\xi})\}\approx 0$ for small s and the main contribution to the integral will come from large s of the order of s_ξ . To solve (1.36) we need to replace the summation by an integral. Going from a discrete sum to a continuous sum does not, of course, create a mathematical identity, unless one takes certain limits. However, when the main contribution from the sum is for large s, it is legitimate to approximate the sum by an integral $\sum \Delta s \approx \int ds$, as we are only interested in the the general scaling behaviour of the system. Thus

$$P(p) \propto \int_{1}^{\infty} s^{1-\tau} \left\{ 1 - \exp(-\frac{s}{s_{\xi}}) \right\} ds. \tag{1.37}$$

One might proceed by integration by parts. You will then discover that only one of the terms are non-zero. However, we will take another approach. We differentiate Eq.(1.37) w.r.t. $1/s_{\xi}$ to find

$$\frac{dP(p)}{d(\frac{1}{s_{\xi}})} \propto \int_{1}^{\infty} s^{2-\tau} \exp(-\frac{s}{s_{\xi}}) ds$$

$$\propto s_{\xi}^{3-\tau} \int_{1/s_{\xi}}^{\infty} z^{2-\tau} \exp(-z) dz \quad \text{substituting } z = s/s_{\xi}.$$

As we are ultimately interested in the limit $p \to p_c$ where the cutoff cluster size diverges, we replace the lower limit $1/s_{\xi}$ with zero and thus

$$P(p) \propto \left(\frac{1}{s_{\xi}}\right)^{\tau-3}$$
 (1.38)

so integrating we find

$$P(p) = c_1 + c_2 \left(\frac{1}{s_{\xi}}\right)^{\tau - 2} \tag{1.39}$$

At $p = p_c$, $s_{\xi} = \infty$. But, $P(p_c) = 0$ implies that $c_1 = 0$. So,

$$P(p) \propto c_2 \left(\frac{1}{s_{\xi}}\right)^{\tau-2},$$

$$\propto |p - p_c|^{\frac{\tau-2}{\sigma}}.$$
(1.40)

Hence, we have derived a new scaling relation

$$\beta = \frac{\tau - 2}{\sigma}.\tag{1.41}$$

By definition

$$P(p) = \begin{cases} 0 & p \le p_c \\ (p - p_c)^{\beta} & p \to p_c^+. \end{cases}$$
 (1.42)

Now we find a third problem with our ansatz 1.

(3) In the derivation above we did not assume $p > p_c$. Thus the ansatz 1 also predicts an infinite cluster for $p < p_c$, which is of course not correct.

Reflecting upon the three problems, we realise that they can all be resolved, as we shall see shortly, by avoiding the argument $s|p-p_c|^{\frac{1}{\sigma}}$ in the scaling ansatz. Thus let us assume the following general scaling form

Ansatz 2

$$n_s(p) = q_0 s^{-\tau} f[q_1(p - p_c)s^{\sigma}] \qquad s \gg 1 \text{ and } p \to p_c.$$
 (1.43)

The scaling ansatz 2 has the following properties:

- q_0 and q_1 are proportionality factors and p_c the critical occupation probability. They all depend on the lattice details. They are non-universal.
- τ , σ are the critical scaling indices which are independent of p, p_c and the lattice structure. They are *universal*.
- f, the scaling function, is independent of p, p_c and detailed lattice structure. It is universal. The precise form of the scaling function f = f(z) has to be determined by computer simulations or other numerical methods since the function f is not predicted by the scaling assumption. Typically, however

$$f(z) = \begin{cases} constant & |z| \ll 1 \Leftrightarrow |p - p_c| s^{\sigma} \ll 1 \Leftrightarrow s \ll |p - p_c|^{-\frac{1}{\sigma}} \propto s_{\xi} \\ decays \text{ fast} & |z| \gg 1 \Leftrightarrow s \gg s_{\xi}. \end{cases}$$
 (1.44)

that is, the scaling function f(z) reaches a constant value (except in 1d percolation theory) for $|z| \ll 1 \Leftrightarrow s \ll s_{\xi}$, and decays rather fast for $|z| \gg 1 \Leftrightarrow s \gg s_{\xi}$. Thus, the role of s_{ξ} as a cutoff and crossover size is maintained. Later, we shall look more carefully at the crossover properties.

- τ , σ and f depend on dimensionality.
- By plotting $\frac{1}{q_0}s^{\tau}n_s(p)$ versus $(p-p_c)q_1s^{\sigma}$, all the data will fall on the universal curve outlining the scaling function f, see Fig. 1.9. This phenomenon is known as *data collapse*.

Problems 7 and 8 highlights some of the points above.

Let us check whether the general scaling ansatz 2 really resolves the three problems associated with the former scaling ansatz 1.

(1) The 1d cluster number distribution

$$n_{s}(p) = (p_{c} - p)^{2} \exp(-\frac{s}{s_{\xi}})$$

$$\approx (p_{c} - p)^{2} \exp(-s(p_{c} - p)) \text{ for } p \to p_{c}$$

$$= s^{-2}(s(p_{c} - p))^{2} \exp(-s(p_{c} - p))$$

$$= s^{-2}f[s^{\sigma}(p_{c} - p)]$$
(1.45)

which is of the form of the general scaling ansatz 2 with $\tau = 2$ and $\sigma = 1$ and $f(x) = x^2 \exp(-x)$. Thus the scaling relation Eq.(1.35) is indeed fulfilled. Note, however, that unlike in higher dimensions, the scaling function increases like x^2 for $x \ll 1$ but that it indeed decays rapidly for $x \gg 1$, see Fig. (1.5).

(2) Keeping s constant we find

$$\frac{\partial^k n_s(p)}{\partial p^k} = q_0 s^{-\tau} f^{(k)} [q_1(p - p_c) s^{\sigma}] q_1^k s^{\sigma k}$$

which is not divergent for $p \to p_c$ assuming that f is analytic, that is, all derivatives of f(z) with respect to z are finite everywhere, also at z = 0.

(3) Let us calculate the strength of the infinite cluster.

$$-P(p) = \sum_{s=1}^{\infty} s n_s(p) - p$$

$$= \sum_{s=1}^{\infty} s n_s(p) - p_c + (p_c - p)$$

$$= \sum_{s=1}^{\infty} [s n_s(p) - s n_s(p_c)] + \mathcal{O}(p - p_c) \quad \text{using } \sum s n_s(p_c) = p_c$$

$$\approx \int_{1}^{\infty} q_0 s^{1-\tau} \left(f[q_1(p - p_c)s^{\sigma}] - f[0] \right) ds$$

Now substitute $z=q_1(p-p_c)s^{\sigma}$. Notice that if $p>p_c$ the argument z is positive while for $p< p_c$ the argument is negative. The cluster size s, however, is always positive so $s=|z|^{\frac{1}{\sigma}}(q_1|p-p_c|)^{-\frac{1}{\sigma}}$ implying that $ds=\frac{1}{\sigma}|z|^{\frac{1}{\sigma}-1}(q_1|p-p_c|)^{-\frac{1}{\sigma}}dz$ with dz positive. Thus we find

$$-P(p) = \int q_0 |z|^{\frac{1-\tau}{\sigma}} (q_1 |p - p_c|)^{\frac{\tau-1}{\sigma}} [f(z) - f(0)]^{\frac{1}{\sigma}} |z|^{\frac{1}{\sigma} - 1} (q_1 |p - p_c|)^{-\frac{1}{\sigma}} dz$$

$$= q_0 (q_1 |p - p_c|)^{\frac{\tau-2}{\sigma}} \int |z|^{\frac{2-\tau}{\sigma} - 1} [f(z) - f(0)]^{\frac{1}{\sigma}} dz.$$
(1.46)

Now it is important to realise that the limits of the integral will depend on the value of p since $z = q_1(p - p_c)s^{\sigma}$. If $p > p_c$, the upper limit will be ∞ (lower limit $p - p_c$ approaches 0 as $p \to p_c^+$) while for $p < p_c$, the lower limit will be $-\infty$ (upper limit approaching 0 as $p \to p_c^-$). Thus if

$$\int |z|^{\frac{2-\tau}{\sigma}-1} [f(z) - f(0)] \frac{1}{\sigma} dz = \begin{cases} \text{constant} \neq 0 & \text{for } p > p_c \\ 0 & \text{for } p < p_c \end{cases}$$
 (1.47)

we have solved the third problem as well, implying

$$P(p) \propto \begin{cases} (p - p_c)^{\beta} & \text{for } p \to p_c^+ \\ 0 & \text{for } p < p_c \end{cases}$$

with

$$\beta = \frac{\tau - 2}{\sigma}$$
.

Exercise 13 Discuss the qualitative behaviour of the scaling function f(z) as a function of $z = q_1(p - p_c)s^{\sigma}$ in order to satisfy the constraint given in Eq.(1.47).

Problem 8 will ask you to calculate the average cluster size S(p) assuming the general scaling ansatz 2.

1.6 Cluster Structure

Till now we have only considered the distribution of cluster sizes and have come up with some useful scaling laws and scaling relations. Now we turn our attention to the geometry of the clusters. We shall do so by mainly studying the *fractal geometry*, which contains information about the density of the clusters on different length scales.

1.6.1 Cluster Radius and Fractal Dimension

Let \mathbf{r}_i denote the position of the *i*th occupied site in a cluster of size s.

Definition 14 The centre of mass of an s-cluster $\mathbf{r}_{cm} = \frac{1}{s} \sum_{i=1}^{s} \mathbf{r}_{i}$.

Definition 15 The radius of gyration R_s of a given s-cluster is defined by

$$R_s^2$$
 = average square distance to the centre of mass
= $\langle |\mathbf{r}_i - \mathbf{r}_{cm}|^2 \rangle$
= $\frac{1}{s} \sum_{i=1}^{s} |\mathbf{r}_i - \mathbf{r}_{cm}|^2$

We want to prove that

$$R_s^2 = \frac{1}{2} \text{ average square distance between two cluster sites} = \frac{1}{2} \frac{1}{s^2} \sum_{ij} |\mathbf{r}_i - \mathbf{r}_j|^2.$$
 (1.48)

By definition, the lefthand side of Eq.(1.48),

$$R_s^2 = \frac{1}{s} \sum_{i=1}^s |\mathbf{r}_i - \mathbf{r}_{cm}|^2$$

$$= \frac{1}{s} \sum_{i=1}^s (\mathbf{r}_i \cdot \mathbf{r}_i + \mathbf{r}_{cm} \cdot \mathbf{r}_{cm} - 2 \mathbf{r}_i \cdot \mathbf{r}_{cm})$$

$$= \frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_i + \frac{1}{s} \sum_{i=1}^s \mathbf{r}_{cm} \cdot \mathbf{r}_{cm} - \frac{2}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_{cm}$$

$$= \frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_i + \mathbf{r}_{cm} \cdot \mathbf{r}_{cm} - 2 \left(\frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \right) \cdot \mathbf{r}_{cm}$$

$$= \frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_i - \mathbf{r}_{cm} \cdot \mathbf{r}_{cm}.$$

Let us rewrite the righthand side of Eq.(1.48)

$$R_s^2 = \frac{1}{2} \frac{1}{s^2} \sum_{ij} |\mathbf{r}_i - \mathbf{r}_j|^2$$

$$= \frac{1}{2} \frac{1}{s^2} \sum_{i=1}^s \sum_{j=1}^s (\mathbf{r}_i \cdot \mathbf{r}_i + \mathbf{r}_j \cdot \mathbf{r}_j - 2 \mathbf{r}_i \cdot \mathbf{r}_j)$$

$$= \frac{1}{2} \frac{1}{s^2} \left[\sum_{i=1}^s s \mathbf{r}_i \cdot \mathbf{r}_i + \sum_{j=1}^s s \mathbf{r}_j \cdot \mathbf{r}_j - 2 \left(\sum_{i=1}^s \mathbf{r}_i \right) \cdot \left(\sum_{j=1}^s \mathbf{r}_j \right) \right]$$

$$= \frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_i - \frac{1}{s^2} (s \mathbf{r}_{cm}) \cdot (s \mathbf{r}_{cm})$$

$$= \frac{1}{s} \sum_{i=1}^s \mathbf{r}_i \cdot \mathbf{r}_i - \mathbf{r}_{cm} \cdot \mathbf{r}_{cm}.$$

The radius of gyration is a more useful quantity to work with since in many situations (like in Polymer Science) we have to deal with more complicated structures than straight lines, squares or spheres.

We also remember that the correlation function $g(\mathbf{r})$ is defined as the probability that a site at a position \mathbf{r} from an occupied site belongs to the same finite cluster. We have the identity

$$\sum_{\mathbf{r}} g(\mathbf{r}) = S(p) \tag{1.49}$$

because the sum is the average number of sites to which an occupied site is connected, see Problem 2.

Definition 16 The correlation length ξ is defined as

$$\xi^2 = \frac{\sum_{\mathbf{r}} r^2 g(\mathbf{r})}{\sum_{\mathbf{r}} g(\mathbf{r})}.$$
 (1.50)

The correlation length represents some average distance of two sites belonging to the same cluster. For a given s cluster, $2R_s^2$ is the average squared distance between two cluster sites. The probability of a site being part of an s cluster is $sn_s(p)$, and it will be connected to s sites (if we include self-connection). The corresponding average over $2R_s^2$ gives the squared correlation length

$$\xi^2 = \frac{\sum_s 2R_s^2 s^2 n_s(p)}{\sum_s s^2 n_s(p)}.$$
(1.51)

The correlation length ξ is the upper cutoff of the radius of those clusters which contribute to the mean cluster size near the percolation threshold. It is expected that ξ diverges as $p \to p_c$, like

$$\xi \propto |p - p_c|^{-\nu}.\tag{1.52}$$

We have introduced a new critical exponent, ν , and we wish to determine how it is related to τ and σ . For 2d percolation, plausible but not rigorous arguments give $\nu = \frac{4}{3}$, in excellent agreement with numerical results. In 3d, ν is somewhat smaller than 0.9, whilst for Bethe lattices one has $\nu = \frac{1}{2}$, analogous to the mean-field theories for thermal phase transitions.

As we have already seen, many quantities diverge at the percolation threshold. Most of these involve sums over all cluster sizes s; their main contribution comes from s of the order $s_{\xi} \propto |p-p_c|^{-\frac{1}{\sigma}}$. Now we see that the correlation length ξ , which is also one of these quantities, is simply the radius of those clusters which contribute the most to divergence. This effect is the foundation of scaling theory. There is one and **only** one length ξ dominating the critical behaviour in an infinite lattice.

1.6.2 Finite Boxing of Percolating Clusters

We now want to find out how the R_s varies with s at the percolation threshold $p = p_c$ where $\xi = \infty$. Let M(L) denote the mass of the percolating cluster within linear distance L. If the percolating cluster was a compact object, then it would be of the form $M(L) \propto L^2$. However, at $p = p_c$, the percolating cluster is a *fractal* object. Figure 1.10 displays the size of the largest cluster S_{∞}

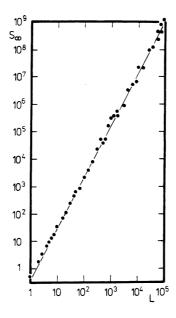


Figure 1.10: The size of the largest cluster S_{∞} at $p = p_c$ as a function of the lattice size L.

(the percolating cluster) as a function of lattice size L in a double-logarithmic plot. The data are consistent with the existence of a fractal dimension D such that

$$M(L) \propto L^D. \tag{1.53}$$

For the 2d case $D = \frac{91}{48} < 2$ and in 1d, D = 1.

Having obtained the relationship in (1.53) it is natural to assume

$$s \propto R_s^D$$
 for $s \gg 1$ at $p = p_c$. (1.54)

Thus,

$$R_s \propto s^{\frac{1}{D}}$$
 for $p \to p_c$. (1.55)

Inserting Eq.(1.55) into Eq.(1.51) we have

$$\xi^{2} \propto \frac{\sum_{s} 2s^{2+\frac{2}{D}} n_{s}(p)}{\sum_{s} s^{2} n_{s}(p)}$$

$$\propto \frac{|p - p_{c}|^{\tau - 3 - \frac{(2)}{D\sigma}}}{|p - p_{c}|^{\tau - 1 - \frac{2}{\sigma}}}$$

$$\propto |p - p_{c}|^{-\frac{2}{D\sigma}}$$

$$\propto |p - p_{c}|^{-2\nu}, \qquad (1.56)$$

where we have used

$$\sum_{s=1}^{\infty} s^k n_s(p) \propto |p - p_c|^{\frac{\tau - 1 - k}{\sigma}}.$$

Therefore we end up with the scaling relation

$$\nu = \frac{1}{D\sigma} \Leftrightarrow D = \frac{1}{\nu\sigma}.\tag{1.57}$$

Note that the behaviour at $p=p_c$ and the behaviour for $s\ll s_\xi$, or $R_s\ll \xi$ are indistinguishable. Therefore, ξ is the crossover length between a critical and noncritical behaviour. On length scales much less than ξ we have $n_s\propto s^{-\tau}$ and $R_s\propto s^{\frac{1}{D}}$ but for length scales much larger than ξ the scaleless behaviour disappears. Note also, that

$$s_{\xi} \propto \xi^{D} \propto |p - p_{c}|^{-\nu D} \propto |p - p_{c}|^{-\frac{1}{\sigma}}$$

confirming once again the scaling relation above between D, ν and σ .

If, however, $p \gg p_c$, the fractal dimension D is expected to be equal to the Eucledian dimension d of the lattice. So,

$$D = d for p > p_c. (1.58)$$

Clusters above p_c are not fractals but 'normal' objects with D=d, provided $s\gg s_{\xi}$ or equivalently $R_s\gg \xi$. Thus s_{ξ} or ξ sets the cluster size and linear scale where there is a crossover from fractal to non-fractal behaviour.

Exponent	1d	2d	3d	4d	5d	6d	Bethe
α	1	-2/3	-0.62	-0.72	-0.86	-1	-1
β	0	5/36	0.41	0.64	0.84	1	1
γ	1	43/18	1.80	1.44	1.18	1	1
ν	1	4/3	0.88	0.68	0.57	1/2	1/2
σ	1	36/91	0.45	0.48	0.49	1/2	1/2
au	2	187/91	2.18	2.31	2.41	5/2	5/2
$D(p=p_c)$	1	91/48	2.53	3.06	3.54	4	4

Table 1.2: The critical exponents for the percolation theory problems in dimensions d = 1, 2, 3, 4, 5, 6 and in the Bethe lattice.

1.6.3 Mass of the Percolating Cluster

Now we wish to see how the scaling relation of the mass M(L) changes for the two different cases.

- (1) For $L \ll \xi$: (always the case at $p = p_c$, where $\xi = \infty$) The percolating cluster appears fractal, implying $M(L) \propto L^D$.
- (2) For $L \gg \xi$: The cluster appear homogeneous

$$\begin{split} M(L) &= \text{ (No. of lattice sites)} \times \text{(Prob. site belongs to percolating cluster)} \\ &= L^d P(p) \\ &= L^d (p-p_c)^\beta \\ &= L^d \xi^{-\frac{\beta}{\nu}} \quad \text{ since } \xi \propto |p-p_c|^{-\nu}. \end{split} \tag{1.59}$$

Now consider $L \approx \xi$, that is, we match the observations above by substituting L with ξ :

$$M(L) \propto L^D \propto \xi^D,$$
 (1.60)

and

$$M(L) \propto L^d \xi^{-\frac{\beta}{\nu}} \propto \xi^{d-\frac{\beta}{\nu}}.$$
 (1.61)

Therefore, we can state that

$$D = d - \frac{\beta}{\nu},\tag{1.62}$$

which is know as a hyperscaling relation because the Euclidean dimension d enters in the scaling relation.

Since the percolating cluster has a constant density for $L \gg \xi$, it is natural to divide the system into boxes of linear size ξ . In d dimensions, the total volume L^d will be divided into $\left(\frac{L}{\xi}\right)^d$ boxes. Since the cluster inside each of these boxes of size ξ^d has a mass of order ξ^D , the total mass of the cluster is given by

$$M(L,\xi) = \left(\frac{L}{\xi}\right)^d \xi^D = \xi^{D-d} L^d, \tag{1.63}$$

which is, of course, equivalent to $P(p)L^d$.

In summary, we have

$$M(L,\xi) \propto \begin{cases} L^D & L \ll \xi \\ \xi^D \left(\frac{L}{\xi}\right)^d & L \gg \xi \end{cases}$$
 (1.64)

which can be written in an alternative form of

$$M(L,\xi) = L^D m(\frac{L}{\xi}), \tag{1.65}$$

where the scaling function

$$m(x) = \begin{cases} \text{constant} & \mathbf{x} = \frac{L}{\xi} \ll 1\\ x^{d-D} & \mathbf{x} = \frac{L}{\xi} \gg 1. \end{cases}$$
 (1.66)

The argument x of the scaling function is a dimensionless number, namely the ratio of the two length scales $\frac{L}{\xi}$. No other length scales play a role. The scaling function describes a crossover from fractal behaviour at length scales L much smaller than the correlation length ξ to uniform behaviour at length scales L much larger than the correlation length ξ . In Nature, there are many examples of crossover phenomena from one type of behaviour to another. Take as an example the table in front of you. On large length scales, the surface of the table is smooth, but going to very small length scales, the surface will become very rough and probably fractal. The mountain range is yet another example. Far away, i.e., on large length scales, it looks pretty smooth, but, as you are well aware, if you are in the middle of the mountain range, on small length scales, it is pretty rough and rugged.

Exercise 14 Give one or two more examples of such crossover phenomena in Nature.

The density has the form

$$\rho(L,\xi) = \frac{M(L,\xi)}{L^d} \propto \begin{cases} L^{D-d} & L \ll \xi \\ \xi^{D-d} & L \gg \xi \end{cases} = L^{D-d} \tilde{\rho}(\frac{L}{\xi}), \tag{1.67}$$

with a scaling function

$$\tilde{\rho}(x) = \begin{cases} \text{constant} & \mathbf{x} = \frac{L}{\xi} \ll 1\\ x^{d-D} & \mathbf{x} = \frac{L}{\xi} \gg 1. \end{cases}$$
 (1.68)

To be aware that the density actually decreases with the length scale when $L < \xi$ can be of immense practical importance. Imagine that you have just been hired by an oil company and you were given a sample of dimensions $0.1 \times 0.1 \times 0.1$ m³ of the porous medium where the oil resides and

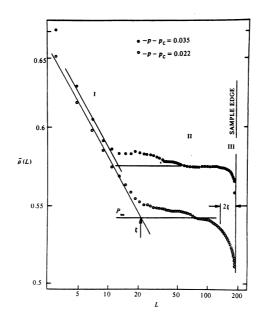


Figure 1.11: The density of sites belonging to the percolating cluster within a region of linear size L. In region I, the ratio $L/\xi \ll 1$ and in region II, $L/\xi \gg 1$. Region III is related to the fact, that the lattices used are finite.

had to estimate how much oil the company could expect to recover in the oil field of dimension, say, $100 \times 100 \times 100 \text{ km}^3$. The percolation model is used as a model for the distribution of oil and gas inside porous rock in oil reservoirs. The empty sites model hard rock while the occupied sites are pores filled with oil. The average concentration of oil is p. Now, if $p < p_c$ there are only finite clusters, so let us assume $p > p_c$. The strength P(p) will be the probability of drilling into a percolating cluster, but how much oil can you recover? You would head for an immediate dismissal if you argued as follows: Measure the density of oil in the sample $\rho(L_1 = 0.1m)$. The mass of oil to be recovered is $M = \rho(L_1 = 0.1m) \cdot (100000m)^3$. The argument is **wrong** simply because the density of oil at length scales $L_2 = 100 \text{ km}$ is **not** given by the density of oil at length scales $L_1 = 0.1 \text{ m}$, see Fig. (1.11). The proper way to argue would be the following: measure the density of oil in the sample $\rho(L_1 = 0.1m) = CL_1^{D-d}$. The density of oil at the reservoir length scale $\rho(L_2 = 100 \text{ km}) = CL_2^{D-d}$ with the same constant C. Taking the ratio we find

$$\rho(L_2 = 100 \text{km}) = \left(\frac{L_2}{L_1}\right)^{D-d} \rho(L_1 = 0.1m)
= \left(10^6\right)^{D-d} \rho(L_1 = 0.1m)
\approx 1.5 \cdot 10^{-3} \rho(L_1 = 0.1m),$$

since in $3d D - d \approx 2.53 - 3 = -0.47$, see table 1.2. The former estimate is wrong by a factor 1000.

1.7 Fractals

The percolating cluster at $p = p_c$ is an example of a random fractal. When $p \neq p_c$ large clusters appear fractal on length scales up to the correlation length $\xi \propto |p - p_c|^{-\nu}$, roughly speaking. In mathematics, we can also encounter deterministic fractals as for example the *Sierpinski carpet* and the *Sierpinski gasket*.

For a geometrical fractal, the mass scales with the linear size raised to the fractal dimension

$$M(L) = L^D \Leftrightarrow D = \frac{\log M(L)}{\log L}.$$

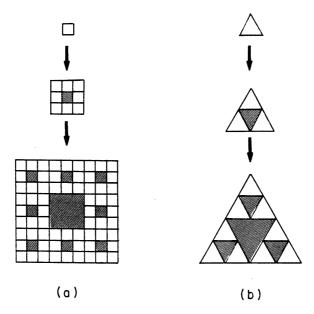


Figure 1.12: Two examples of deterministic fractals. (a) The Sierpinski carpet. The first three levels in the algorithm for constructing the Sierpinski carpet are shown. The linear scale is enlarged by a factor 3 with the condition that an occupied square (white) is replaced with with 3×3 squares in which the centre square is empty (grey) while an empty square (grey) is replaced with 3×3 empty squares. (b) The Sierpinski gasket. A similar algorithm generates the Sierpinski gasket.

Let n denote the iteration number. By inspection of the Sierpinski carpet, $M=8^n$ and $L=3^n$, implying

$$D = \frac{\log 8^n}{\log 3^n} = \frac{\log 8}{\log 3} \approx 1.893.$$

In the case of the Sierpinski gasket, $M=3^n$ and $L=2^n$, yielding

$$D = \frac{\log 3}{\log 2} \approx 1.585.$$

Note that if the length scale is rescaled by a factor b, then

$$M(\frac{L}{b}) = \left(\frac{L}{b}\right)^D = \frac{L^D}{b^D} = \frac{M(L)}{b^D}$$

so that the mass is reduced by a factor b^D . Using this observation as the characteristic of fractal behaviour for random fractals we can easily find, say, the scaling of the mass of the percolating cluster $M(L,\xi)$ as a function of L and ξ . Let us rescale the length scales by a factor b, that is, $L \to \frac{L}{b}$ and $\xi \to \frac{\xi}{b}$ (no other length scales are present). Thus

$$\begin{split} M(L,\xi) &= b^D M(\frac{L}{b},\frac{\xi}{b}) \\ &= b^D b^D M(\frac{L}{b^2},\frac{\xi}{b^2}) \\ &\vdots \\ &= b^{Dl} M(\frac{L}{b^l},\frac{\xi}{b^l}). \end{split} \tag{1.69}$$

If we are at the critical point $p = p_c$, $\xi \propto |p - p_c|^{-\nu} = \infty$, but then $\frac{\xi}{b^l} = \infty \ \forall l$. If we stop the above renormalisation procedure when $b^l = L$ we find

$$M(L, \xi = \infty) = \left(b^l\right)^D M\left(\frac{L}{b^l}, \frac{\xi}{b^l} = \infty\right)$$

$$= L^D M(1, \infty)$$

$$= L^D.$$
(1.70)

This proves that self-similarity is mathematically expressed by power-law behaviour. Now, assume $p>p_c$ with $\xi\propto |p-p_c|^{-\nu}<\infty$ with

$$M(L,\xi) = b^{Dl} M(\frac{L}{b^l}, \frac{\xi}{b^l}).$$

We now have to consider two cases depending on the ratio L/ξ .

(a) If $L/\xi \ll 1 \Leftrightarrow L \ll \xi$ (which is allways the case at $p = p_c$) we stop the iteration process when we reach the smallest length scale $b^l = L$ and we "recover"

$$M(L,\xi) = L^D M(1,\frac{\xi}{L}) = L^D M(1,\infty) \propto L^D.$$

(b) If $L/\xi \gg 1 \Leftrightarrow L \gg \xi$, we stop the iteration process when $b^l = \xi$ and we find

$$M(L,\xi) = \xi^D M(\frac{L}{\xi}, 1) \propto \xi^D \left(\frac{L}{\xi}\right)^d = \xi^{D-d} L^d,$$

since for a uniform system $M(\frac{L}{\xi}, 1) \propto (\frac{L}{\xi})^d$.

Exercise 15 Discuss why the system looks uniform when $\xi/b^l=1$.

1.8 Finite-size scaling

Let us consider the percolation problem for $p \neq p_c$ where the correlation length is finite

$$\xi \propto |p - p_c|^{-\nu} \Rightarrow |p - p_c| \propto \xi^{-\frac{1}{\nu}}$$
.

The strength of the infinite cluster for $p > p_c$ can then be expressed in terms of the finite correlation length

$$P(p) \propto (p - p_c)^{\beta} \propto \xi^{-\frac{\beta}{\nu}}$$

and similarly for the average cluster size

$$S(p) \propto |p - p_c|^{-\gamma} \propto \xi^{\frac{\gamma}{\nu}}.$$

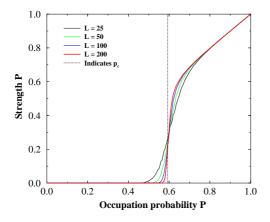
These are the results in infinite lattices with $L = \infty$. Now, what happens at finite lattice sizes when $L < \infty$? Well, nothing happens as long as $L \gg \xi$. The only relevant length scale is the

correlation length ξ . However, when $L \ll \xi$, the length scale will be set by L. This we have already encountered before, we just didn't stress that point. Better late that never:

$$\begin{split} P(L,\xi) &= \rho(L,\xi) \\ &= \frac{M(L,\xi)}{L^d} \\ &= \begin{cases} L^{D-d} & L \ll \xi \\ \xi^{D-d} & L \gg \xi. \end{cases} \\ &= \begin{cases} L^{-\frac{\beta}{\nu}} & L \ll \xi \\ \xi^{-\frac{\beta}{\nu}} & L \gg \xi. \end{cases} \\ &= \xi^{-\frac{\beta}{\nu}} f(\frac{L}{\xi}) \end{split}$$

where the scaling function

$$f(\frac{L}{\xi}) = \begin{cases} \left(\frac{L}{\xi}\right)^{-\frac{\beta}{\nu}} & \frac{L}{\xi} \ll 1\\ \text{constant} & \frac{L}{\xi} \gg 1. \end{cases}$$



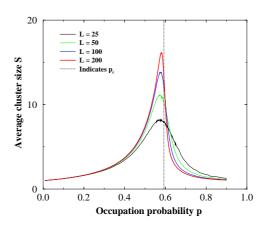


Figure 1.13: (a) The strength P(p) measured in a 2d square lattice for finite system sizes as a function of occupation probability p. When p is far away from p_c , $L \gg \xi$ and the strength is determined by $\xi^{-\frac{\beta}{\nu}}$. However, with p closer to p_c , the finite-size effect is seen and P(p) decays with system size as $L^{-\frac{\beta}{\nu}}$. (b) The average cluster size S(p) measured in a 2d square lattice for finite system sizes L as a function of occupation probability p. When p is far away from p_c , $L \gg \xi$ and the average cluster size is determined by the correlation length $\xi^{\frac{\gamma}{\nu}}$. However, with p closer to p_c , the finite-size effect is seen and S(p) increases with system size as $L^{\frac{\gamma}{\nu}}$.

Similarly for the average cluster size, we would expect

$$S(L,\xi) \propto \left\{ \begin{array}{ll} L^{\frac{\gamma}{\nu}} & L \ll \xi \\ \xi^{\frac{\gamma}{\nu}} & L \gg \xi. \end{array} \right.$$

Generally, if we have a quantity

$$X \propto |p - p_c|^{-\chi} \propto \xi^{\frac{\chi}{\nu}}$$
 for $L \gg \xi$

then we would expect

$$X(L,\xi) \propto \begin{cases} L^{\frac{\chi}{\nu}} & L \ll \xi \\ \xi^{\frac{\chi}{\nu}} & L \gg \xi. \end{cases}$$
$$= \xi^{\frac{\chi}{\nu}} x_1(\frac{L}{\xi}) \tag{1.71}$$

or, in terms of occupation probabilities

$$X(L,p) = |p - p_c|^{-\chi} x_2 (L^{\frac{1}{\nu}}(p - p_c)).$$

The important message we get is that by studying *finite-size scaling*, that is, studying X as a function of (finite) system sizes L at $p = p_c$, we can extract the exponent $\frac{\chi}{u}$.

1.9 Real space renormalisation in percolation theory

Imagine a percolation lattice with n sites. The total number of different microscopic configurations is 2^n as a site can be in one of two states – occupied with probability p or empty with probability 1-p. Table (1.3) shows the number of microscopic configurations in a two dimensional square lattice of linear size L.

L	1	2	3	4	5	6	7	8	9	10	17	100
n	1	4	9	16	25	36	49	64	81	100	289	10000
2^n	2	16	512	65536	$3 \cdot 10^7$	$7 \cdot 10^{10}$	$6 \cdot 10^{14}$	$2 \cdot 10^{19}$	$2 \cdot 10^{24}$	10^{30}	10^{87}	10^{3000}

Table 1.3: The number of microscopic configurations 2^n as a function the linear size L of a two-dimensional square lattice where $n = L^2$, the number of sites in the lattice. For lattice size L = 17, the number exceeds the estimated number of atoms in the universe $\approx 10^{81}$.

In principle, if we wanted to calculate the average of a quantity $\langle A \rangle$ (say the average cluster size), we should evaluate the quantity A_i associated with each configuration i and then weight the quantity A_i with the probability p_i (which would be of the form $p^m(1-p)^{(n-m)}$, where m is the number of occupied sites in that particulate configuration) of the system to be in that microscopic state, that is,

$$\langle A \rangle = \frac{\sum_{i} p_{i} A_{i}}{\sum_{i} p_{i}} = \sum_{i} p_{i} A_{i}. \tag{1.72}$$

This procedure, however, soon becomes an impossible task due to the numbers of different states involved. With today's computing power one might do, say, a 7×7 system, but an 8×8 system would take approximately 40 years on a tera flop (10^{12} calculations per second) while the time required to do a 10×10 system would exceed the age of the universe which is approximately $15 \cdot 10^9$ years.

Real space renormalisation is a *coarse graining* procedure where we systematically reduce the number of degrees of freedom (sites) in order to break a large problem down into a sequence of smaller and more manageable stages by eliminating fluctuations on scales less than a given length scale b. The effect will be to reveal the large scale behaviour of the system.

Before we introduce the real space renormalisation method, let us make some observations related to the phase transition in a percolation model.

(a) The empty state at occupation probability p = 0 is self-similar with an associated correlation length $\xi = 0$.

- (b) The fully occupied state at occupation probability p = 1 is self-similar. The associated correlation length $\xi = 0$. The ordered state has an order parameter P(p = 1) = 1.
- (c) The states at the critical occupation probability $p = p_c$ are also self-similar and the correlation length $\xi = \infty$. The infinite cluster is fractal and looks alike on all length scales and we have clusters of all sizes from s = 1 to $s = \infty$.

Loosely speaking, the correlation length ξ sets the scale of the largest fluctuation from the "averaged" state. For $p \neq p_c$, the correlation length is identified with the linear size of the cutoff cluster size s_{ξ} .

When $p < p_c$ the upper cutoff of the linear size of the fluctuations away from the empty state is given by ξ and when p approaches zero, ξ approaches zero. At p = 0, there are no clusters left at all and $\xi = 0$.

When $p > p_c$, the correlation length can also be identified with the upper cutoff in the linear size of the largest holes in the percolating (spanning) cluster which indicates how far away you are from the fully occupied state. When p approaches one, ξ approaches zero. At p = 1, there are no holes left and $\xi = 0$.

At the phase transition point $p = p_c$, the correlation length is infinite. Thus there are fluctuations from the smallest length scale up to infinity.

The real space renormalisation technique is based on the so-called *block site (spin) technique* introduced by Leo Kadanoff and later formalised into the renormalisation group method by Kenneth Wilson, who received the Nobel price in 1982 for "his theory for critical phenomena in connection with phase transitions", see, for example, the website on physics laureates http://www.nobel.se/physics/laureates/

The renormalisation group method has three basic steps:

- 1. Divide the lattice into blocks of linear size b (in terms of the lattice constant) with each block containing a few sites (spin).
- 2. Next, the coarse graining procedure takes place. The sites in the blocks are averaged in some way (to be specified more precisely shortly) and the entire block is replaced by a single super site (spin) which is occupied with a probability according to the renormalisation group transformation $p' = R_b(p)$.
 - In the combined procedure 1 and 2, one should keep the symmetry of the original lattice such that we can repeat the coarse graining procedure again. The result of these two operations are to create a new lattice whose fundamental spacing is b times as large as the original lattice.
- **3.** Restore original lattice constant by rescaling the length scales by the factor b.

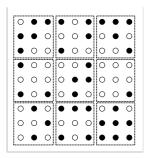
These 3 steps define a renormalisation group transformation R_b , where the number of degrees of freedom is reduced drastically. Note that it is called a group because of the property that when applying the transformation to a configuration $\{s_i\}$,

$$R_{b_2}(R_{b_1}(\{s_i\})) = R_{b_1b_2}(\{s_i\}) \tag{1.73}$$

but it is of course not a group in a strictly mathematical sense because no inverse transformation exists since we are reducing the number of degree of freedom.

The effect of the coarse graining procedure in step 2 is to eliminate from the system all fluctuations whose scale is smaller than the block size b. Any small scale fluctuations of the sites over a range of less than b lattice units will be smeared out. This is somewhat similar to the process taking place if you view the system through a lens out of focus – all the smaller features are blurred but the large scale features are unaffected.

Let us clarify the 3 steps by looking at a simple example. Consider a 2d square lattice with 9×9 sites, that is, 81 degrees of freedom and a total of $2^{81} = 2 \cdot 10^{24}$ different configurations.



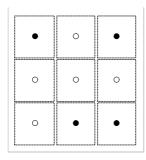




Figure 1.14: The three renormalisation group steps illustrated in a 2d square lattice with b=3. The majority rule defines the renormalisation group transformation.

- 1. Divide the square lattice up into small 3×3 blocks with a total of 9 sites (b = 3)
- 2. We now have to specify the course graining procedure which will define the renormalisation group transformation. One possibility would be to use the so-called **majority rule** which states that if a majority of the sites in the block is occupied, then the super site should be occupied, otherwise empty. The probability, that a majority of sites are occupied in the 3×3 block then defines the renormalisation group transformation

$$p' = R_b(p) = p^9 + K_{9.1}p^8(1-p) + K_{9.2}p^7(1-p)^2 + K_{9.3}p^6(1-p)^3 + K_{9.4}p^5(1-p)^4$$

where $K_{9,k}$ is the number of different ways to place k empty sites into the cells of 9 sites. The super site should be occupied with probability $p' = R_b(p)$ and empty with probability $1 - p' = 1 - R_b(p)$.

3. Rescale the lattice of super sites by a factor 3 to restore original lattice constant.

Let ξ denote the correlation length in the original lattice. Assume we are close to p_c . Then

$$\xi = \text{constant} |p - p_c|^{-\nu} \tag{1.74}$$

We denote the correlation length in the new renormalised lattice by ξ' . Since the length scales have been rescaled by a factor b (step 3)

$$\xi' = \frac{\xi}{b} \Leftrightarrow$$

$$\operatorname{constant} |R_b(p) - p_c|^{-\nu} = \frac{\operatorname{constant} |p - p_c|^{-\nu}}{b}$$

$$(1.75)$$

where $R_b(p)$ is the renormalisation group transformation that determines the new occupation probability in the rescaled lattice associated with the new (smaller as b > 1) correlation length.

Simple rearranging implies that

$$\left(\frac{|R_b(p) - p_c|}{|p - p_c|}\right)^{-\nu} = \frac{1}{b}$$
(1.76)

so the critical exponent ν is given by

$$\nu = \frac{\log b}{\log\left(\frac{|R_b(p) - p_c|}{|p - p_c|}\right)}.$$
(1.77)

The basic idea is that at the critical point p_c we have self-similarity, that is,

$$\xi' = \xi. \tag{1.78}$$

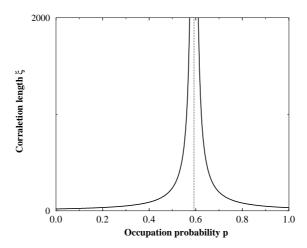


Figure 1.15: When renormalising the length scales by a factor b, the correlation length decreases unless it was 0 or ∞ initially. Associated with a decrease in the correlation length is a flow in occupation probability space either towards p=0, if initially $p < p_c$ or towards p=1, if initially $p > p_c$. The fixed points of the renormalisation group transformation are associated with the trivial self-similar states at p=0 or p=1 or the nontrivial self-similar states at $p=p_c$.

This equation can only be consistent with Eq.(1.76) if

$$\xi = \begin{cases} \infty \\ 0. \end{cases} \tag{1.79}$$

This is intuitively clear as $\xi = 0$ is associated with either p = 0 (empty lattice) or p = 1 (fully occupied lattice) the two trivially self-similar cases and $\xi = \infty$ with the critical point p_c . Furthermore, we can also conclude that

$$\xi = \text{constant } |p - p_c|^{-\nu} = \xi' = \text{constant } |R_b(p) - p_c|^{-\nu}$$
 (1.80)

which implies that the phase transition $\xi = \infty$ is identified with (one of) the fixed points p^* of the renormalisation group transformation, that is, the solutions of the equation

$$R_b(p^*) = p^*. (1.81)$$

Thus

$$\frac{|R_b(p) - p_c|}{|p - p_c|} = \frac{|R_b(p) - R_b(p_c)|}{|p - p_c|}$$

$$= \frac{dR_b(p_c)}{dp} \text{ for } p \to p_c \tag{1.82}$$

leaving, see Eq.(1.77)

$$\nu = \frac{\log b}{\log\left(\frac{dR_b(p_c)}{dp}\right)} \tag{1.83}$$

1.9.1 Renormalisation group transformation in 1d.

Consider a renormalisation group transformation in 1d. Take a 1d lattice where each site is occupied with probability p. Divide the lattice into blocks with p sites. Let the renormalisation group

transformation be determined by the probability of having a spanning cluster. The probability of having a spanning cluster in a block of b sites is

$$R_b(p) = p^b$$
.

The fixed point equation can easily be solved

$$R_b(p^*) = p^{*b} = p^* \Leftrightarrow p^* = \begin{cases} 0\\ 1. \end{cases}$$

If we start with an empty lattice p=0, the renormalised lattice will also be empty, associated with the fixed point $p^*=0$. If we start with a fully occupied lattice p=1, the renormalised lattice will also be fully occupied since all the blocks contain a percolating cluster, associated with the fixed point $p^*=1$. However, if we start with a lattice containing some empty sites p<1, the renormalised lattice will contain even more empty sites because $p'=R_b(p)=p^b< p$. Repeating the renormalisation procedure will gradually bring the renormalised occupation probability towards zero. Clearly, $p^*=0$ is associated with $\xi=0$, while $p^*=1$ is associated with $\xi=\infty$ and must thus be identified with the critical occupation probability p_c .

Furthermore, in order to calculate the correlation length exponent ν we need to take the derivative of the renormalisation group transformation evaluated at $p^* = 1$.

$$\frac{dR_b(p)}{dp}|_{p^*=1} = bp^{b-1}|_{p^*=1} = b,$$

implying

$$\nu = \frac{\log b}{\log \frac{dR_b(p)}{dp}|_{p^*=1}} = 1,$$

so in 1d the renormalisation group transformation is exact.

1.9.2 Renormalisation group transformation on 2d triangular lattice.

Divide the lattice into triangular cells containing three sites each. Let the probability for having a spanning cluster define the renormalisation group transformation. Thus

$$R_b(p) = p^3 + 3p^2(1-p) = 3p^2 - 2p^3. (1.84)$$

The fixed point equation

$$R_b(p^*) = 3p^{*2} - 2p^{*3} = p^* \Leftrightarrow p^* = \begin{cases} 0 \\ 1 \\ 1/2. \end{cases}$$

The two trivial fixed point is associated with the self-similar states of an empty lattice and fully occupied lattice. The unstable fixed point $p^* = 1/2$ will be associated with the nontrivial self-similar states at p_c . The critical exponent ν is

$$\nu = \frac{\log b}{\log \frac{dR_b(p)}{dp}|_{p^*=1/2}} = \frac{\log \sqrt{3}}{\log (6p - 6p^2)|_{p^*=1/2}} = \frac{\log \sqrt{3}}{\log 3/2} = 1.355.$$

The exact values are $p_c = 1/2$ and $\nu = 4/3$ so the renormalisation group transformation does a good job.

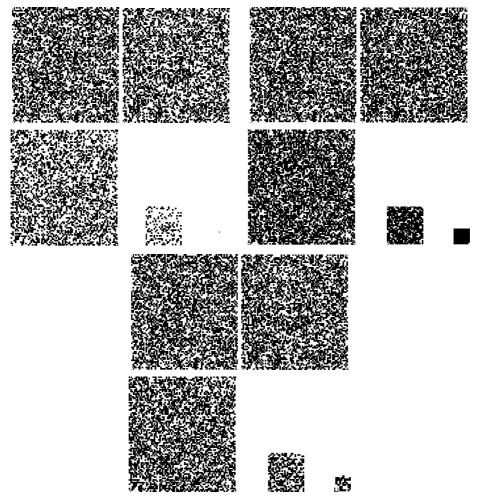


Figure 1.16: Renormalisation group method on a 2d square lattice according to the majority rule for 3×3 blocks. Shown are part of the original lattice L = 729 and the renormalised lattices L = 243 (part of), L = 81, 27, and 3. (a) Initial occupation probability $p < p^*$ in the original lattice and the flow is towards the empty lattice. (b) Initial occupation probability $p > p^*$ in the original lattice and the flow is towards the fully occupied lattice. (c) Initial occupation probability $p = p^*$ in the original lattice. This is a fixed point for the renormalisation group transformation and consequently there is no flow. It looks like itself on all length scales.

1.9.3 Renormalisation group transformation on 2d square lattice of bond percolation.

Consider the block defined in Fig. (1.17) which, after the coarse graining procedure, is replaced by two superbonds. The renormalisation group transformation is

$$p' = R_b(p)$$

= probability to have a spanning cluster in horizontal direction
= $p^5 + p^4(1-p) + 4p^4(1-p) + 2p^3(1-p)^2 + 2p^3(1-p)^2 + 4p^3(1-p)^2 + 2p^2(1-p)^3$
= $2p^5 - 5p^4 + 2p^3 + 2p^2$ (1.85)

with the fixed point equation

$$R_b(p^*) = 2p^{*5} - 5p^{*4} + 2p^{*3} + 2p^{*2} = p^* \Leftrightarrow p^* = \begin{cases} 0\\1\\1/2. \end{cases}$$

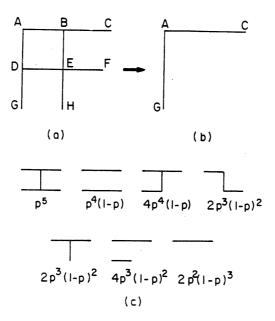


Figure 1.17: Renormalisation group method of 2d square lattice with bond percolation according to the spanning cluster rule. (a) and (b) After the coarse graining procedure, the block is replaced with two super bonds AC and AG. (c) The various configurations with a horizontal spanning cluster. The two dangling bonds DG and EH need not be considered as they do not affect the probability of having a spanning cluster from left to right.

Again, the two trivial fixed points are associated with the self-similar states of an empty lattice and fully occupied lattice. The unstable fixed point $p^* = 1/2$ will be associated with the nontrivial self-similar states at p_c . For bond percolation in 2d, $p_c = 1/2$, see Table 1.1. The critical exponent ν is

$$\nu = \frac{\log b}{\log \frac{dR_b(p)}{dp}|_{p^* = 1/2}} = \frac{\log 2}{\log 13/8} = 1.428,$$

which should be compared to the analytical result of $\nu=4/3$ in 2d. Thus the renormalisation group transformation defined above for bond percoaltion in 2d results in an exact prediction of p_c and a good estimate of ν .

1.9.4 Why is the renormalisation group transformation not exact?

There are two significant sources of error which is the reason for not obtaining the exact results

- (1) Two sites that were connected in the original lattice can be disconnected and vica versa.
- (2) The renormalised system is not really a **true** percolation system because the probabilities of having bonds between supersites are no longer independent. As we shall see later, this is the equivalent of introducing next-nearest-neighbour couplings in the renormalisation group procedure in the 2d Ising model. Thus we should really introduce new parameters but we choose here to truncate the problem to only one parameter, the occupation probability p.

Glossary

Taken from The New Physics ed. Paul Davies, Cambridge University Press.

Coarse-graining An operation implementing some form of spatial averaging which smoothes out relatively small length scale configurational structure while preserving the larger length-scale structures

Correlation length The correlation length ξ gives a measure of the typical length scale over which fluctuations of one microscopic variable are correlated with the fluctuations of another. In percolation theory, it is the typical cluster diameter of the clusters s_{ξ} which give the main contribution to the divergence of the second (and higher) moments of the cluster distribution. Close to a critical point $\xi \propto |p-p_c|^{-\nu}$ for $p \to p_c$.

Critical phenomena The phenomena which occur in the neighbourhood of a continuous (second order) phase transition, characterised by very long correlation lengths.

Critical exponents (or indices) Near a critical point, physical quantities are often proportional to a power of another quantity, such as the distance from the critical point $|p-p_c|$. The power that occurs known as a critical exponent (index).

Critical point A point in a phase diagram, where the correlation length associated with the physical system is, in principle, infinite.

Fractal geometry Generalisation of Euclidean geometry suitable for describing irregular and fragmented patterns such as the percolating cluster at $p = p_c$. A noninteger **fractal dimension** D can frequently be associated with such patterns.

Order parameter A variable such as the strength of the infinite cluster in percolation theory (or the magnetisation in an Ising model) used to describe the degree of order in a phase above (below) its critical point. In a continuous phase transition (second order phase transition), the order parameter goes continuously to zero as the critical point is approached from above (below).

Phase transition A change of state such as occurs in the boiling or freezing of a liquid, or in the change between ferromagnetic and paramagnetic states of a magnetic solid. An abrupt change, characterised by a jump in an order parameter is known as first order; a change in which the order parameter evolves smoothly to or from zero is called continuous or second order.

Renormalisation group In statistical physics, the renormalisation group method systematically implement some form of coarse-graining operation (e.g. rescaling length scales with a factor b: $L \to \frac{L}{b}, \xi \to \frac{\xi}{b}$) to expose the character of the large-scale phenomena, in systems where many length scales are important.

Scale invariance A physical system is said to exhibit scale-invariance if it remains unchanged (in a statistical sense) by a coarse-graining operation.

Universality The phenomena whereby many microscopically quite different physical systems exhibits critical point behaviour, with quantitatively identical features, such as critical exponents. In percolation theory e.g. the critical exponents do not depend on the microscopic details of the lattice but only on the Euclidean dimension d.

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