

THESIS
2
2000



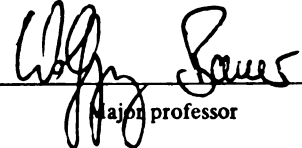
This is to certify that the
thesis entitled
Phase Transitions in a
Two-Component Site-Bond Percolation Model

presented by

Holger M. Harreis

has been accepted towards fulfillment
of the requirements for

M. S. degree in Physics


Major professor

Date August 20, 1999

LIBRARY
Michigan State
University

PLACE IN RETURN BOX to remove this checkout from your record.
TO AVOID FINES return on or before date due.
MAY BE RECALLED with earlier due date if requested.

DATE DUE	DATE DUE	DATE DUE

Phase Transitions in a Two-Component Site-Bond Percolation Model

By

Holger Martin Harreis

A THESIS

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

MASTER OF SCIENCE

Department of Physics and Astronomy

1999

ABSTRACT

Phase Transitions in a Two-Component Site-Bond Percolation Model

By

Holger Martin Harreis

In standard percolation models either bond (randomly open edges) or site (randomly occupied vertices) percolation is dealt with. Site-bond percolation combines the two formulations, dealing with randomly occupied sites and randomly existing bonds connecting these sites. However in this version of the model only one active component exists, the other sites are considered unoccupied. A further generalization is to consider several components, which was done for site percolation as well as bond percolation previously and called polychromatic percolation.

In this work, a method to treat a N -component percolation model as effective one component model is presented by introducing a scaled control variable p_+ . In Monte Carlo simulations on 16^3 , 32^3 , 64^3 and 128^3 simple cubic lattices the percolation threshold in terms of p_+ is determined for $N = 2$. Phase transitions are reported in two limits for the bond existence probabilities p_+ and p_- . In the same limits, empirical formulas for the percolation threshold p_+^c as function of one component-concentration, f_b , are proposed. In the limit $p_- = 0$ a new site percolation threshold, $f_b^c \simeq 0.145$, is reported.

ACKNOWLEDGEMENTS

First of all I wish to express my most grateful thanks to Professor Wolfgang Bauer for giving me the opportunity to come to Michigan State University and work in his research group at the NSCL as well as for his being my advisor during this wonderful year.

I profoundly appreciated the very friendly atmosphere in the NSCL Nuclear Theory Group in particular and at the NSCL in general. Furthermore I am indebted to Sen Cheng, Jens Höfkens and Jens von Bergmann for numerous conversations. In particular it is a pleasure to acknowledge the fruitful discussions led with Jens von Bergmann and the answers that Jens Höfkens provided to all computer related questions.

I appreciated the financial support by the German National Scholarship Foundation, the Studienstiftung des deutschen Volkes.

Contents

LIST OF TABLES	vi
LIST OF FIGURES	vii
1 Introduction	1
2 The Foundations of Percolation Theory	3
2.1 Percolation Models	3
2.1.1 Bond Percolation	4
2.1.2 Site Percolation	6
2.1.3 Site-Bond Percolation	8
2.1.4 Polychromatic Percolation	9
2.1.5 Miscellaneous Percolation Models	10
2.2 Phase Transitions	13
2.2.1 Definitions	13
2.2.2 The Order Parameter	15
2.2.3 The Correlation Length and Long Range Order	16
2.2.4 Critical Exponents and Universality	18
2.2.5 The Thermodynamic Limit	21
2.3 Monte Carlo Simulations	22
2.4 Some Results	23
2.4.1 The Infinite Cluster	23
2.4.2 Cluster Size	28
2.4.3 The Number of Open Clusters per Vertex	30
2.4.4 Cluster Numbers	31
2.4.5 Scaling Theory	38
2.4.6 Analogies of Percolative Phase Transitions to Thermal Phase Transitions	43
2.5 Finite Size Scaling	43

2.6	Percolation in Nuclear Physics	47
3	Two-Component Site-Bond Percolation	50
3.1	General Case: N Components	50
3.2	Two Components using the Natural Variables	52
3.2.1	General Considerations	53
3.2.2	Simulation Results	54
3.3	Simulation Techniques	56
3.3.1	General Features	56
3.3.2	Cluster Analysis	58
3.3.3	Determination of the Critical Value	59
3.4	Two Components using the Scaled Control Parameter	61
3.4.1	Entire Parameter Range	62
3.5	The Percolation Probability	69
3.5.1	$p_{\neq} \rightarrow 0$ Limit	69
3.5.2	The 'Smearing-Out' Effect	77
3.5.3	$p_{=} \rightarrow 0$ Limit	78
3.6	The Critical Value of the Scaled Control Parameter	82
3.6.1	$p_{\neq} \rightarrow 0$ Limit	82
3.6.2	$p_{=} \rightarrow 0$ Limit	84
3.6.3	Concentration Dependence in the $p_{\neq} = 0$ Limit	85
3.6.4	The Cut-Out Technique	90
3.6.5	Concentration Dependence in the $p_{=} = 0$ Limit	92
3.7	Finite Size Effects	96
3.7.1	One-Dimensional Percolation Model	96
3.7.2	Techniques in Higher Dimensions	97
3.7.3	A Proposal for a Novel Technique	101
3.8	Spin-Off Results	103
3.8.1	The Number of Open Clusters per Vertex	103
3.8.2	The Number of Spanning Clusters per Vertex	104
3.8.3	Two-Dimensional Percolation	106
4	Summary and Conclusion	109
A	Source Code	112
A.1	perc_prob_00.f	112
A.2	perc_ppintv0477.f	122

List of Tables

2.1	Critical exponents in a ferromagnetic system (d is the dimension of the system under observation)	19
2.2	Percolative functions and their analogous counterpart in thermal systems.	43
2.3	Percolative functions and the section in which they were first introduced or further discussed.	43

List of Figures

2.1	Example of a typical site percolation configuration on a square lattice in the subcritical phase. Black squares represent occupied vertices. . .	7
2.2	Example of a typical site percolation configuration on a square lattice in the subcritical phase. Black squares represent occupied vertices. . .	8
3.1	Probability to belong to the infinite cluster, p_∞ , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_ =$ and p_\neq , calculated for a fraction of the blue species of $f_b = 0.5$	54
3.2	Probability to belong to the infinite cluster, p_∞ , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_ =$ and p_\neq , calculated for a fraction of the blue species of $f_b = 0.2$	55
3.3	Probability to belong to the infinite cluster, p_∞ , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_ =$ and p_\neq , calculated for a fraction of the blue species of $f_b = 0.0$	55
3.4	Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter, p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, for values of $p_ =, p_\neq \in [0, 1]$, fitted with $p_\infty \propto (p_+ - p_+^c)^\beta$ (solid line). Here $p_+^c \simeq 0.251$ for the 'upper' branch, $p_+^c \simeq 0.280$ for the 'lower' branch and $\beta = 0.41$ in both cases. The inset shows the same data in a double logarithmic representation.	62
3.5	Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter, p_+ , in a 128^3 simple cubic lattice with $f_b = 0.3$, for values of $p_ =, p_\neq \in [0, 1]$, fitted with $p_\infty \propto (p_+ - p_+^c)^\beta$ (solid line). Here $p_+^c \simeq 0.251$ for the 'upper' branch, $p_+^c \simeq 0.218$ for the $p_\neq = 0$ branch, $p_+^c \simeq 0.266$ for the $p_ = = 0$ branch and $\beta = 0.41$ in all cases.	66
3.6	The same data as shown in Fig. 3.5 in a double logarithmic representation, with a slope of all three curves of $\beta = 0.41$	67
3.7	The normalized density of edges connecting two sites of equal flavor, $\alpha_=(f_b)$ and the normalized density of edges connecting two sites of different flavor, $\alpha_\neq(f_b)$. See also (3.14) and (3.15).	68

3.8	Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_- = 1$ for varied p_\neq . 50 independent simulation events where taken into account and the average was taken over events in which the number of br -bonds actually formed in the simulation, n_{br} , was non-zero.	74
3.9	Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_- = 1$ for varied p_\neq . 50 independent simulation events where taken into account and the average was taken over all events. .	75
3.10	Percolation probability as a function of p_\neq , with a parametric dependence on p_+ , shown for a 128^3 simple cubic lattice with $f_b = 0.5$	78
3.11	Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_\neq = 1$ for varied p_- . 50 independent simulation events where taken into account and the average was taken over events in which the number of br -bonds actually formed in the simulation, n_{br} , was non-zero.	82
3.12	Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.5$, plotted as a function of p_\neq	83
3.13	Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.5$, plotted as a function of p_-	85
3.14	Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.3$, plotted as a function of p_\neq	86
3.15	Critical value of the scaled control parameter, p_+^c , plotted as a function of the fraction of blue sites, f_b , in the limit $p_\neq = 0$ and obtained from simulations on simple cubic lattices of size $L = 16^3$, $L = 32^3$, $L = 64^3$ and $L = 128^3$ by a fit to the scaling law $ p_+^c(L) - p_+^c \propto L^{-1/\nu}$. The errors, estimated as described in [vdM97], are smaller than the symbol sizes.	87
3.16	Threshold p_-^c versus concentration f_b for two one-component site-bond percolation models.	89
3.17	Threshold p_+^c versus concentration f_b for two one-component site-bond percolation models.	90
3.18	Percolation probability p_∞ versus the probability that a site gets 'cut-out', p_{cut}	91
3.19	Critical value of p_\neq and of the scaled control parameter, p_\neq^c and p_+^c , plotted as a function of the fraction of blue sites f_b in the limit $p_- = 0$. The data has been obtained by a fit to $ p_+^c(L) - p_+^c \propto L^{-1/\nu}$. Again the errors, estimated as described in [vdM97], are smaller than the symbol sizes.	93

3.20	Exact (solid line) and approximative (dashed line) effective threshold in a one-dimensional percolation system as a function of the linear lattice dimension L	98
3.21	Finite size scaling for $p_+^c(L, p_{\neq} = 0)$ shown as a function of the linear dimension of a simple cubic lattice at a concentration of the blue species of $f_b = 0.5$	99
3.22	Probability ψ that a spanning cluster exists, versus the lattice size L . The percolation threshold p_+^c is given by the common intersection point $\psi_{L_{max}}(p_+^c)$	101
3.23	The number of open clusters per vertex in a simple cubic 128^3 lattice, calculated for a concentration of the blue species $f_b = 0.5$. Also shown is the approximate theoretical expectation.	104
3.24	Probability to belong to the infinite cluster, $p_{\infty}(p_+)$, and the probability to belong to any percolating cluster, $p_{pc}(p_+)$ in a simple cubic 100^3 lattice at $f_b = 0.5$	106
3.25	Threshold p_-^c versus concentration f_b for two one-component site-bond percolation models on the square lattice, compare Fig. 3.16.	107

Chapter 1

Introduction

Critical phenomena are an everyday experience, not only in laboratories, but even more in kitchens around the world do they have quite some importance in applied experiments. Whoever has boiled an egg, whoever has made water boil (or freeze) has let a phase transition happen. The theory of phase transitions has evolved to a very important tool. A general feature of phase transitions is the fact that some quality of the system under observation changes when a parameter which is freely adjustable, is changed. The freezing of water or boiling of an egg are examples of phase transitions in which the quality undergoing a transition changes abruptly as a function of the varied external parameter. Here, this quality is the microscopic structure, or, related to that, the density. Two distinct phases are present and are separated, if one plots, for example, the density ρ versus the temperature T in a phase diagram, by the phase transition line, on which, when 'crossed', the system goes from one phase to another. In the 1940's, research on polymers and the process of polymerization led to the question how the phase diagram for polymers might look like and how one might find a reasonably simple model for polymerization that yet would be able to reproduce the qualitative characteristics of such a complex system as a polymer solution. The process of polymerization is close to the 'hardening' of an egg while being boiled: Single molecules, or monomers, form larger and larger

macromolecules, large, but finite clusters of monomers, by means of an increasing number of chemical bonds. Such a viscous solution of branched polymers is called *sol* and it may result, at some point, in a very large network, of size on the order of the system size, called a *chemical gel* (Physical gels in contrast are formed by means of reversible bonds such as in the gelation of silica particles in water or NaCl solutions). Examples of such sol-gel transitions in everyday life are pudding, gelatine or the milk-to-cheese transformation. The first model to describe the behavior of gelation was essentially invented by Flory, [Flo41], and Stockmayer, [Sto43], in 1941 and 1943. In 1957, Broadbent and Hammersley, [BH57], introduced the term 'percolation' and a more mathematical approach to the model. In subsequent papers, the percolation model has been applied, in a broad diversity of techniques, to a very wide range of problems, see [Sah94], such as dispersion and flow in porous media, fracture and fault patterns in rock, the morphological and transport properties of composite materials, conductivity of (semi-) conductors, reaction kinetics, antigen-antibody reactions and aggregations as well as the network formation on lymphocyte membranes.

In this work we will give, in Chapter 2, an introduction to some basic concepts of percolation and statistical models and then present a multi-component site-bond percolation model in Chapter 3. The results of Monte-Carlo simulations of this model in the special case of two components will also be shown. In the same chapter, two limits of the two component site-bond percolation model will be dealt with and their characteristics discussed.

We shall furthermore abide by the following notation: Words defined in the text will be emphasized using *italic font*, words considered to be important for the particular section will be highlighted by means of **bold font**.

Chapter 2

The Foundations of Percolation Theory

In percolation theory, in the most general case, one deals with a graph of dimension d without a priori specifying a certain structure. In this discussion, however, we will restrict ourselves to percolation theory on the graph associated with \mathbb{Z}^d and more specifically, we will only discuss $d = 3$ in most cases.

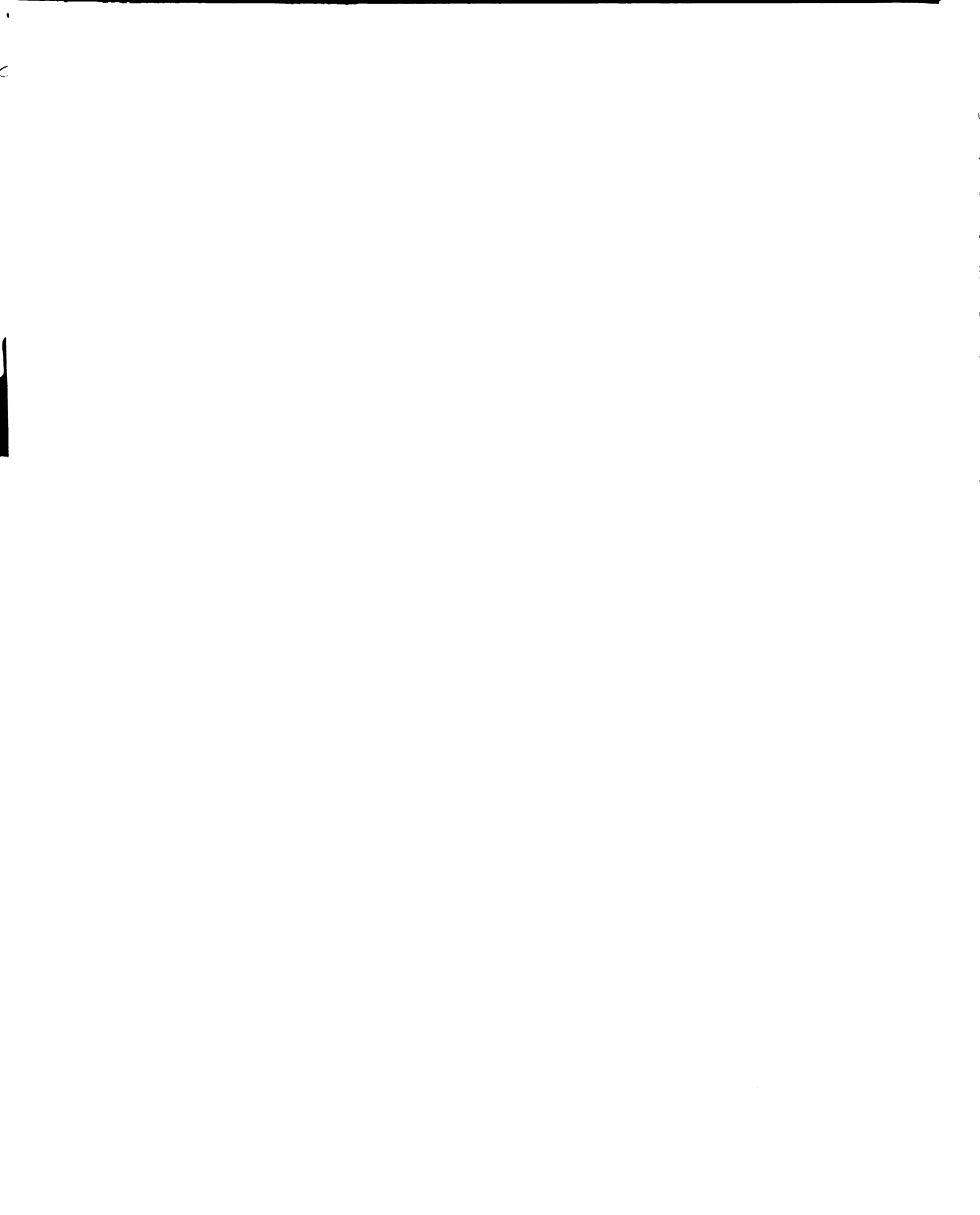
2.1 Percolation Models

Let us begin with yet another illustrating example. We imagine a very large porous rock that we submerge in a pool. At its center we have installed a water sensor. What is the probability that the water will find its way to the center of the stone and wet our sensor? To answer the question, we might try to model this random medium, the stone, in the following way. Let p be a number that satisfies $0 \leq p \leq 1$ and \mathbb{Z}^3 be the simple cubic lattice. We then walk through the lattice and assign, at random, with probability p , a bond to each edge (called *open edge*), whereas with probability $(1 - p)$ we leave the edge unoccupied (*closed edge*). After this we analyze the structure on the lattice by deleting the closed edges, which leaves us with all open edges and the set of their endpoints. All sites that are at least singly connected by bonds are said

to belong to one cluster. The question of the sensor-wetting is now related to the existence of an *infinite cluster*. Clearly, in a finite system, which we will always have to work with in a simulation, it is not at all apparent what infinite should mean, we will come back to this question in the following sections, here it is sufficient to think of it as a cluster that spans the whole system. It is easy to imagine that with increasing p also the size of the clusters increases. At some point p_c however, we will have an abrupt change in the structure: An infinite cluster will exist in the lattice for $p > p_c$ and the wetting of the center of the rock becomes possible. This value of p is called the critical value or the percolation threshold. The model presented here has bonds as the main ingredient and is thus called the *bond percolation model*. We will introduce it in more depth in the following section, accompanied by an introduction to other formulations of percolation models in the next sections. We will then present results of percolation theory, which in most cases will generally hold for bond and site percolation.

2.1.1 Bond Percolation

We shall write $\mathbb{Z} = \{\dots, -1, 0, 1, \dots\}$ for the set of all integers and \mathbb{Z}^d for the set of all integral coordinate vectors $z = (z_1, z_2, \dots, z_d)$ where d is the dimension of the system. The integral coordinate vectors z shall be called *vertices*. We call \mathbb{E}^d the set of all line segments $\langle x, y \rangle$, (*edges*), between a pair of vertices x and y . Vertices and edges together form the *lattice*, denoted by \mathbb{L}^d , which, in the case of $d = 3$ is the simple cubic lattice. Let p and q satisfy $0 \leq p \leq 1$ and $p + q = 1$. We shall assign each edge the condition *open* with probability p and the condition *closed* with probability q . An equivalent formulation shall be to state that an edge is occupied by a bond or unoccupied. Furthermore the assignments shall happen uncorrelated, each edge is open or closed independently of all others. By $P_p(X)$ we shall denote the probability



of some event X and we will write $E_p(A)$ for the expectation value of an observable A . A *path* of length m in the lattice \mathbb{L}^d means a sequence $z_0, e_0, z_1, e_1, \dots, z_{m-1}, e_{m-1}, z_m$ of vertices z_i and open edges $e_i = \langle z_i, z_{i+1} \rangle$. A *circuit* of length $m + 1$ shall mean a path z_0, e_0, \dots, z_m satisfying $e_m = \langle z_m, z_0 \rangle$. Path and Circuit are called open if all of their edges are open, and closed if all of their edges are closed. A *subgraph* of \mathbb{L}^d is a set of edges e_i and vertices z_i with $e_i \in \mathbb{E}^d$ and $z_i \in \mathbb{Z}^d$. Two subgraphs are *disjoint* if they do not have any edge and vertex in common, they are *edge-disjoint* if none of their edges is an element of both subgraphs. With the definition of a subgraph we can finally put up the following definition: An *open cluster* or just *cluster* is every subgraph that first only consists of open edges and the vertices connected to them and secondly is disjoint from all other such subgraphs. To specify a particular cluster we will write $C(z)$, indicating that it contains the vertex z and it will mean the set of vertices connected to z through open paths. The *size* of a cluster $C(z)$ will be written as $|C(z)|$ and is defined as the number of vertices contained in $C(z)$. A cluster of size one would then be just one vertex without any open edge: $C(z) = \{z\}$. If we furthermore introduce the notation $z \longleftrightarrow y$ to indicate that there exists an open path joining vertex z and vertex y , than a cluster may also be written as $C(z) = \{y \in \mathbb{Z}^d : z \longleftrightarrow y\}$. In the same spirit, $z \not\longleftrightarrow y$ means that there exists no open path connecting z and y . Finally, the *surface* of a cluster C will be denoted by ∂C and is defined as the set of vertices in C that are adjacent to vertices not in C . In the definitions made here, for example in defining a cluster, we have assumed that we only deal with nearest neighbor interaction. This is not a necessary condition, percolation models with connections even longer than next-nearest neighbors have been introduced, see 2.1.5. For a connection range that goes to infinity, however, the percolation threshold goes to zero.

2.1.2 Site Percolation

Site percolation may be formulated in an analogous way to bond percolation. Again, we consider \mathbb{Z}^3 and call the integral coordinate vector $z \in \mathbb{Z}^d$ a vertex. We also add the set of edges \mathbb{E}^d to obtain the *lattice* \mathbb{L}^d . As before, we need two random variables, f and g which, again, shall satisfy $0 \leq f \leq 1$ and $f + g = 1$. However now, the objects of interest are not the edges, which are open with probability p and closed with probability q in the bond percolation model, but rather the **vertices** which in the site percolation model are assigned the quality *open* with probability f and *closed* with probability $g = (1 - f)$. Every edge is considered to be open, closed vertices can be thought of as junctions that are blocked. With this notion we can use the concept of a *path* and a *circuit* as introduced above. Also the definition of a *cluster* as given in the previous section still holds. Furthermore, no change is necessary in the definitions of *size* and *surface* of a cluster. We show an example of typical site percolation configurations on the square lattice in Figs. 2.1 and 2.2, where occupied sites are represented by black squares, whereas unoccupied sites are symbolized by white squares. An experiment that was actually carried out and for which the shown site percolation problem on the square lattice can be seen as a model, is to place conducting and non-conducting spheres in a bowl and check on percolation as a function of the concentration of the conducting spheres. In Fig. 2.1 we show the system with a relatively low concentration of conducting spheres and we can see that the system is in a non-conducting state, there is no path of black squares that leads through the entire lattice. The system is in a *subcritical state*. In Fig. 2.2 the system is shown at a higher concentration of black squares, that is at a higher concentration of conducting spheres. As can be seen, a percolating path that spans the entire lattice, exists. The system is found to be in a *supercritical state*. Obviously some transition takes place in the lattice in between these two states. The question

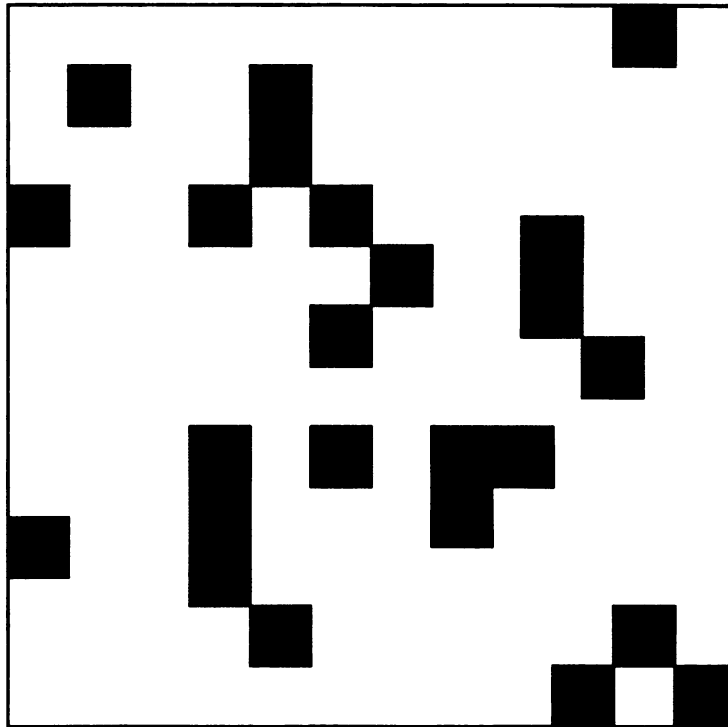


Figure 2.1: Example of a typical site percolation configuration on a square lattice in the subcritical phase. Black squares represent occupied vertices.

is, how this transition happens in detail.

As already briefly stated at the end of 2.1, many results hold for bond and site percolation. A more strict way is to say that the bond percolation and the site percolation model belong to the same universality class, [Sta79], meaning that they are described by the same set of critical exponents, which will be introduced in Sec. 2.4. Still, although bond percolation was historically first, site percolation is the more general of the two models, since it is known that every bond percolation process on a given lattice can be expressed in terms of a site model on a different lattice, see, for example, [Fis61], [FE61] and [Kes82]. The converse statement, however, does not hold generally.

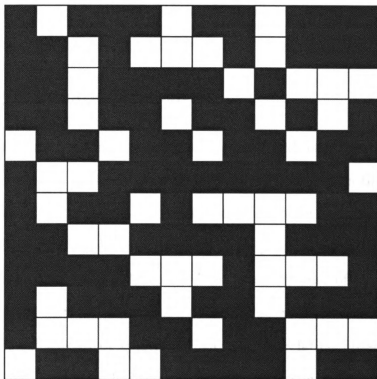


Figure 2.2: Example of a typical site percolation configuration on a square lattice in the subcritical phase. Black squares represent occupied vertices.

2.1.3 Site-Bond Percolation

A very natural generalization of the two previous models is to simultaneously allow open and closed edges as well as open and closed vertices. This means that no longer only edges determine the 'passage' of percolation as in the bond model, or only sites do so, as in the site percolation model, but rather both the condition of edges and vertices becomes important. We then have $p, q \in [0, 1]$ with $p + q = 1$ and simultaneously $f, g \in [0, 1]$ satisfying $f + g = 1$. The concept of a cluster is still valid as in the two models presented before. Both models from Secs. 2.1.1 and 2.1.2 represent certain limits of the site-bond percolation model: Bond percolation is site-bond percolation with $f = 1$ fixed and site percolation is site-bond percolation in the limit $p = 1$. The site-bond percolation model thus allows us to go continuously from bond to site

percolation and vice versa. As cited in [Sta79], some of the earlier work on site-bond percolation can be found in [OCG⁺78, WP78, CSK79, ARRS79].

2.1.4 Polychromatic Percolation

If one does not think of each vertex to be associated with only two states, occupied or unoccupied, one has, in the most general formulation, N states the vertex can be in, of which one can think of as an occupation by different species. Zallen, [Zal77] introduced such a generalization for bond and site percolation and also gave it the name *polychromatic percolation*. He focused on the coexistence of percolating species in highly connected lattices, giving a criterion for the occurrence of a panchromatic regime in which all species percolate and showing percolation phase diagrams. In such a generalized model one has several 'percolation systems' on one lattice and if the appropriate parameters are favorable, one can, in principle, have all 'systems' percolating. One important parameter is the connectivity of the lattice. On the simple cubic lattice, for example, with a coordination number $Z = 6$ (again only counting nearest neighbors), percolation of both species is possible in a certain range of the bond existence probability p or the fraction of sites f , but on the square lattice with $Z = 4$, no such regime exists. Therefore, not only the structure, but also the dimension of the lattice is important in polychromatic percolation. Yet another version of polychromatic percolation has been introduced by Halley and Holcomb, [HH78]. They considered a so called 'Three-Component Reactive Percolation Model'. The essentials are as follows: Two types of atoms are considered which can furthermore react and form dimer molecules. Each vertex in the lattice can be occupied by either one type of the atoms or the molecule. The main focus lies on the resistivity, which was shown to behave qualitatively the same as observed in experiments.

A further generalization of polychromatic percolation lies in applying it to the

site-bond percolation model, thus dealing with N different types of vertices and a corresponding number of different edges, given by the number of combinations in which neighboring vertices can occur. Work on this problem has been carried out in the context of nuclear physics, see Sec. 2.6, [Baued], with two components, and in a general approach for N components, where an approximate percolation criterion was given, in [Ios95]. Further work has been done in the frame of this thesis and we will deal with this problem in a later part of this work in further detail.

2.1.5 Miscellaneous Percolation Models

A variety of further different models have been proposed over the years, of which we want to briefly introduce some, without giving a detailed review of every model.

Long-Range Interaction

In our discussion a cluster has been defined as the set of vertices and edges that are connected by nearest-neighbor distances only. It is also possible to work with longer range interactions. If one lets the coordination number z go to infinity, however, the percolation threshold goes to zero as $1/(z - 1)$. As stated in [Sta79], in work with nearest and next-nearest neighbor interactions on bcc lattices, [HSB⁺79, QBH76], as well as with higher order interactions, [HKM78], no differences from ordinary percolation have been found, indicating that also taking longer range interactions into account does not change the universality class of the model.

Percolation on the Cayley Tree

This model is also called percolation on the Bethe lattice. It presents a very special case, which nonetheless has received some attention, as the percolation problem is exactly solvable here. In the Bethe lattice, one starts with one point, the origin and

adds z neighbors to it, out of which z neighbors emanate again, one of which is the connection to the origin, but $z - 1$ are new sites. Thus no closed loops are possible. It turns out that in the high dimensionality limit, $d \rightarrow \infty$, percolation on hypercubic lattices can be approximatively described by percolation on the Bethe lattice, since in higher dimensions loops on hypercubic lattices become increasingly unimportant.

Trees on a Lattice

Analogously to the Bethe lattice, one can constrain percolation on other lattices to be 'non-cyclic', which causes a different behavior to emerge than the one observed in ordinary percolation. As stated in [Sta79] no phase transition occurs in the case of the square lattice.

Interacting Percolation

Until now, we have considered percolation to be an uncorrelated random process, meaning that the state of each edge or vertex was completely independent of the state of all of its neighbors. We may introduce some correlation by combining percolation models with the Ising model of ferromagnets. One possible realization is, for example, the so called Ising-correlated site-bond percolation discussed in [HS81]. In this model the sites are occupied not randomly but correlated as the spins in an Ising model and then bonds are formed with a certain bond existence probability, which gives three free parameters: The site concentration f , the temperature T and the bond existence probability p . Random site-bond percolation is still contained as $T \rightarrow \infty$ limit in this model (And thus also ordinary bond and site percolation in the $f \rightarrow 1$ and $p \rightarrow 1$ limits respectively).

Continuous Percolation

All discussed percolation models so far happened to be constrained to a lattice of some structure (we focused on the lattices related to \mathbb{Z}^d), processes in nature however take place in continuous systems. Therefore the question arises, if critical exponents turn out to be different in percolation processes that take place in a random model system with continuous variables. Numerical evidence seems to exist that, at least in three dimensions, the lattice structure is not important for the critical exponents. Also considerations from the renormalization approach are in favor of this statement.

Directed Percolation

In this version of percolation, one can exclude open edges in some directions, allowing only bonds to exist in the other directions. This will make the percolation threshold go up. A further discussion can be found in the literature, for example [Dua90].

Invasion Percolation

One can think of invasion percolation as a system to dynamically model the displacement of one fluid by another in a random medium as, for example porous rock. The model uses a lattice where each site is assigned a number $r \in [0, 1]$ representing the radius of the pore, which a vertex is considered to model. All edges are open and represent the throats. According to the fact that capillary forces dominate, an advancement of the invading fluid to pores with small radius takes place. One thus starts out with all sites occupied by the defending fluid, the invading fluid is injected from one site of the lattice. In each step, the neighboring defending fluid sites with the smallest radius are occupied by the invading fluid. Finite clusters of the defending fluid that are completely disjoint from the rest of the fluid can form. They give rise to two different versions of the model: Either the defending fluid is modeled as

incompressible (like oil, for example) and the invading fluid can not advance in those trapped finite clusters of the defending fluid, or it is modeled as compressible and the invading fluid can further advance. In both cases the advancement stops as soon as the invading cluster has reached the opposite site of the sample and percolates. One then has the system at its critical point always. Systems exhibiting this feature are called 'self-organized critical', [BC89]. No finite clusters of the invading fluid exist and one does not have an equivalent of the occupation probability f . It turns out that in the former case, that is with trapping, invasion percolation is different from ordinary percolation, whereas for invasion percolation without trapping the results are equivalent to ordinary percolation.

2.2 Phase Transitions

Before, in Sec. 2.4, we will arrive at a discussion of some important results of percolation theory, we want to briefly review a few aspects of phase transitions in general, as well as, in Sec. 2.3, give a concise presentation of Monte-Carlo simulation techniques.

2.2.1 Definitions

A variety of physical phenomena can be seen as belonging to two categories. Systems in the first category are characterized in that their constituents do not interact with each other or that at least the interaction is negligible. In this case a knowledge of the energy level of all the constituents allows a direct calculation of the thermodynamic functions of the entire system. Examples of phenomena belonging to this first category are the specific heat of gases and solids, where for the solids the interaction is a priori not negligible but since for a very wide range of temperature the positions of the atoms stay more or less fixed in space, a transformation to normal coordinates is possible so that the entity of atoms can essentially be treated as a system of (practically)

non-interacting harmonic oscillators. Another example is the spectral distribution of black-body radiation. Systems belonging to the second category, however, do not provide the basis for such a simple calculation of the thermodynamic functions, one can not eliminate the interaction by means of any transformation. This interaction leads, at some value of the temperature or another parameter, to a macroscopically significant form of *cooperative behavior*. As a result, the thermodynamic functions of systems in this category exhibit analytic discontinuities or singularities which are associated with the phenomenon of *phase transitions*. Prominent examples are the melting of solids, the condensation of gases, the phenomena of ferromagnetism and antiferromagnetism, order-disorder transitions as well as normal state to superfluid and normal state to superconducting state transitions.

Fundamental is the notion of a *phase*, it means a possible state of a macroscopical system in thermal equilibrium. In different phases, the same macroscopical observables of the same system can assume totally different values, depending on the values of external parameters. Regions in the parameter space in which changes of these parameters bring forth a change of the system from one phase into the other, are the critical parameter ranges.

The earliest classification of phase transitions was provided in 1933 by Ehrenfest, in which the *order* of a phase transition is the means of classification. An *n-th order phase transition* is, following Ehrenfest, characterized in that the $(n - 1)$ st first partial derivatives of the free enthalpy G after the natural variables of the system (i.e. the temperature T and the pressure p in the fluid system or the temperature and magnetic field in the case of the magnet) are continuous at the transition point, whereas the n th derivative exhibits a discontinuity at this point. With increasing order, however, the differences between two phases grow increasingly unimportant and the question arises to which order a distinction between two phases is possible.

Furthermore it turns out that phase transitions who are not of first order type are characterized rather by singularities than by discontinuities as the Ehrenfest theory would imply. There are other reasons, that go beyond the scope of this brief review, that have led to the conclusion that the Ehrenfest scheme does not allow for a classification general enough. That is why the Ehrenfest classification scheme has been more or less abandoned, only two types of phase transitions remain: *Discontinuous phase transitions* and *continuous phase transitions*, where the former correspond to the first order phase transitions in the Ehrenfest classification and the latter essentially represent the second order phase transitions in a broader sense. The definition of the discontinuous phase transition remains as for the first order phase transitions. They are characterized by discontinuities in the first partial derivatives of some thermodynamic potentials (i.e. discontinuities in the volume or in the spontaneous magnetic moment). A continuous phase transition is present if there is non-analytical behavior observed in the second partial derivatives at the critical point (e.g. experimentally in the response functions like the heat capacity, the compressibility or the susceptibility). In most cases however, the notation remains according to the old classification, with 'first order phase transition' and 'second order phase transition' used.

A phenomenological approach for a unified description of all second order phase transitions was given by Landau, we will just refer to the literature, for example [Pat96].

2.2.2 The Order Parameter

We already cited the non-analytical behavior at a critical point as being characteristic for a continuous phase transition. Aside this effect, a further typical characteristic of a continuous phase transition is the *order parameter*. It signifies a macroscopic observable that only makes sense to define in one of the two phases in a phase tran-

sition. The name arises since phase transitions are often associated with a change in the order of the system. In a multi-particle system there are always two 'competing' tendencies for minimizing the free energy $F = U - T S$: To minimize the internal energy U , which can be achieved by a high order state, or to maximize the entropy S , which goes along with a higher order state of the system. The effect of the entropy however, scales linearly with temperature and thus the equilibrium will be temperature dependent, which can lead to a phase transition, separating two phases characterized by different order states of the system. Examples of order parameters are:

- Ferromagnet: Spontaneous magnetization $M_s = m_s/V$.
 $(m_s: \text{Magnetic moment}), \text{ with } M_s \begin{cases} > 0, & \text{if } T < T_c \\ = 0, & \text{if } T > T_c \end{cases}$
- Gas-Liquid system: Density difference $\Delta n = n_f - n_g$.

For $T < T_c$ there are two phases, gas and liquid with two different densities n_f and n_g , whereas above T_c there is just one homogeneous phase where it makes no sense to define Δn .

2.2.3 The Correlation Length and Long Range Order

An important concept in the context of phase transitions is the *correlation function* of an observable A , being defined in the following way:

$$g(\vec{r}, \vec{r}') = \langle a(\vec{r})a(\vec{r}') \rangle - \langle a(\vec{r}) \rangle \langle a(\vec{r}') \rangle, \quad (2.1)$$

where $a(\vec{r})$ is the density of A :

$$A = \int d^3r a(\vec{r}). \quad (2.2)$$

The correlation function gives a measure of how much correlated the physical property A is at \vec{r} and at \vec{r}' . In a spatially homogeneous system we have that the correlation

function is invariant under translations and thus becomes

$$g(\vec{r}, \vec{r}') = g(|\vec{r} - \vec{r}'|).$$

As an example, let us consider the density correlation

$$g_n(\vec{r}, \vec{r}') = \langle n(\vec{r})n(\vec{r}') \rangle - \langle n(\vec{r}) \rangle,$$

where $n(\vec{r})$ means the particle density. In the special case of a homogeneous system one usually encounters a damped, oscillatory behavior of g as a function of the distance $|\vec{r} - \vec{r}'|$, with vanishing correlations for $|\vec{r} - \vec{r}'| \rightarrow \infty$:

$$g_n(|\vec{r} - \vec{r}'|) \xrightarrow{|\vec{r} - \vec{r}'| \rightarrow \infty} 0.$$

This happens, since for increasing distance the first term in (2.1) factorizes:

$$\langle n(\vec{r})n(\vec{r}') \rangle \xrightarrow{|\vec{r} - \vec{r}'| \rightarrow \infty} \left(\frac{N}{V}\right)^2.$$

Generally, the behavior of the correlation function in the vicinity of a critical point is conjectured to follow:

$$g(\vec{r}, \vec{r}') \propto \frac{\exp\left(\frac{|\vec{r} - \vec{r}'|}{\xi(T)}\right)}{|\vec{r} - \vec{r}'|}. \quad (2.3)$$

This can be taken as a heuristic defining equation for the *correlation length* $\xi(T)$.

It obviously sets a length scale in the system, giving a measure for the range of the correlation. A very important property of the correlation length is that it diverges at the critical point:

$$\xi(T) \xrightarrow{T \rightarrow T_c} \infty. \quad (2.4)$$

This implies, that when approaching the critical point, the correlation length will grow above the range of every interaction range in the system, spatial correlations

from microscopic constituents will assume macroscopic dimension. One speaks of *long-range order* or also *critical fluctuations*. The most important implication of this behavior is that the physical properties of the system will, in the regime of critical fluctuations, no longer be determined by the microscopic form of the interaction or structure, but rather by the value of the correlation length ξ , so that different observables of entirely different systems can show remarkably qualitatively equal behavior in the vicinity of their respective critical points. This phenomenon is known as *universality*. Furthermore the system is *scale-invariant*, it 'looks' the same, no matter on what level of magnification it is looked at.

2.2.4 Critical Exponents and Universality

Very often, one observes the following limiting behavior of some physical property A in the vicinity of a critical point. A shows a power law dependence on a reduced parameter ε . The reduced parameter ε is obtained from the parameter τ which leads to the phase transition:

$$\varepsilon = \frac{\tau - \tau_c}{\tau_c}, \quad (2.5)$$

where τ_c denotes the critical value of the parameter τ . ε then determines the critical behavior according to

$$A(\varepsilon) \underset{\varepsilon \rightarrow 0}{\propto} \varepsilon^\psi. \quad (2.6)$$

This introduces a *critical exponent* ψ which determines the behavior in the direct vicinity of the critical point. In the sense of the discussion in Sec. 2.2.3 and the implications given by the divergence of the correlation length, a power law is to be expected since at the critical point the system loses any characteristic length scale: A power law does not introduce a characteristic length scale, as for example opposed to an exponential behavior $\propto e^{x/a}$, where a would set a length scale. As there are

some physical quantities, like, for example, the heat capacity in the Ising model, that diverge logarithmically on approaching the critical point and not according to a power law, a critical exponent is usually defined in a more general way:

$$\psi = \lim_{\varepsilon \searrow 0} \frac{\ln |A(\varepsilon)|}{\ln \varepsilon} \quad (2.7)$$

$$\psi' = \lim_{\varepsilon \nearrow 0} \frac{\ln |A(\varepsilon)|}{\ln \varepsilon}. \quad (2.8)$$

In this definition the power law is contained as a special case. It is not a priori clear that the same exponent $\psi = \psi'$ should hold for approaching the critical point from both sides. In Table 2.1 we have compiled the critical exponents that usually appear in a ferromagnetic system, see [Nol98]. The Greek letters used here are convention. For simplicity we have omitted the primed exponents. The exponent η seems, at first

Property	Exponent	Definition		
Heat Capacity	α	$C_H \propto \varepsilon^{-\alpha}$	$\varepsilon \rightarrow 0$	$H = 0$
Order Parameter	β	$M_s \propto -\varepsilon^\beta$	$\varepsilon \nearrow 0$	$H = 0$
Susceptibility	γ	$\chi_T \propto \varepsilon^{-\gamma}$	$\varepsilon \rightarrow 0$	$H = 0$
Critical Isotherm	δ	$M \propto H^{1/\delta}$	$\varepsilon = 0$	$H \rightarrow 0$
Correlation Length	ν	$\xi \propto \varepsilon^{-\nu}$	$\varepsilon \rightarrow 0$	$H = 0$
Correlation Function	η	$g(\vec{r}, \vec{r}') \propto \vec{r} - \vec{r}' ^{-d+2-\eta}$	$\varepsilon = 0$	$H = 0$

Table 2.1: Critical exponents in a ferromagnetic system (d is the dimension of the system under observation)

sight, to have no real implication, since in (2.3) the behavior of $g(\vec{r}, \vec{r}')$ at the critical point was already given. From there, η should, since $\xi \xrightarrow{\varepsilon \rightarrow 0} \infty$, simply be given by $\eta = 3 - d$. η however provides a means to quantify how much a real physical system deviates from the simple conjecture in (2.3).

As already briefly stated in the previous section, a most remarkable feature of continuous phase transitions is the phenomenon of *universality*. Since in discontinuous phase transitions the correlation length stays finite and does not diverge, critical

phenomena, along with universality are only observed in continuous phase transitions. The concept of universality was introduced by Griffiths, [Gri70]. The *universality hypothesis* states that the critical exponents are nearly universal, that is to say, they are nearly the same for all thermodynamical systems. They only depend on

1. the dimension d of the system
2. the range of the interaction-potential in the system
3. the spindimensionality n .

For a classification of the interaction-range the interaction potential is usually assumed to follow a functional form as

$$V(r) \propto r^{-(d+2+f)},$$

where r is the inter-particle distance. For $f > 0$ one then speaks of a *short-ranged* interaction, if $f < (d/2) - 2$, then the interaction is said to be *long-ranged* and for $(d/2 - 2) < f < 0$ one speaks of *medium-ranged* interaction. In the first case, real universal behavior is expected, the interaction range is negligible compared to the diverging correlation length. In the second case, the classical theories with a special set of critical exponents become correct and in the third case one has to deal with a rather complicated situation, where the critical exponents may depend on the actual value of f . The spindimensionality gives the number of independent degrees of freedom of the spins in the system. For example, $n = 1$ in the Ising model, $n = 2$ in the XY model and $n = 3$ in the Heisenberg model.

The critical exponents are not independent, but rather show mutual dependencies, which are manifested in the *scaling laws*. It turns out that there exist two independent critical exponents, through which all others can be expressed. These are mostly results

of *renormalization theory*, to which we will briefly come back at a later point in the context of finite-size scaling in percolation theory.

2.2.5 The Thermodynamic Limit

Thermodynamic potentials of a macroscopic system are known to be extensive,

$$(\propto N, \propto V),$$

meaning that at constant temperature, the total energy of the system can be seen as a sum of the energies of parts of the system. This however requires that the interaction between particles in one part and particles in another be negligible, which can rigorously be only true in the thermodynamic limit

$$N \rightarrow \infty, V \rightarrow \infty, \text{ such that } \frac{N}{V} \rightarrow \text{const.} \quad (2.9)$$

Also only in the thermodynamic limit do the predictions of the different statistical descriptions, canonical, microcanonical and grandcanonical ensemble coincide.

Furthermore, and this is the most important result for a discussion of phase transitions, it can be shown that in a rigorous sense, in a finite system, no phase transitions are possible. As example, one can contemplate a classical N -particle system in the volume V . Thermodynamic potentials involve the logarithm of the grandcanonical partition function Λ . Phase transitions should then be expected at the zeros of Λ . The grandcanonical partition function Λ turns out to be a polynomial of order N' with one-particle canonical partition functions Z_i as parameters, which are all positive definite (N' is the maximum number of particles to fit in V). Thus for $N' < \infty \iff V < \infty$ there can occur no phase transition in the system. A detailed theory has been developed by Yang and Lee, see for example [Pat96, Nol98].

2.3 Monte Carlo Simulations

In investigating thermal systems one will almost never, aside from some special situations, encounter an exactly solvable problem. The Ising model, for example, is exactly solvable, but only up to two dimensions and for some special lattices. In most of the cases, thus, in order to calculate an observable, one will have to rely on some other technique than direct calculation since the number of possible configurations in a typical system forbids any practical analytical approach. Furthermore, such a calculation would be rather inefficient, as a high number of configurations does essentially not contribute to the expectation value of the observable since their probability is negligible. That is, one will have to use numerical methods. In most cases then one will not include the whole configuration space \mathbb{S} in the averaging, but just some finite portion of it, depending on the precision one wants to achieve. The most desirable way to sample the configuration space, would be to include all those configurations that contribute with a higher probability than others at the given temperature. This procedure is called *importance sampling*. It is realized in an algorithm by defining a transition function $P(\phi|\pi)$. It gives the conditional probability that one configuration $\phi \in \mathbb{S}$ is changed to some other configuration $\pi \in \mathbb{S}$. This function has to fulfill the following requirements that we only want to cite but not discuss in further detail, see [Bin79, BH97] for a discussion. It shall be *ergodic*, provide for *detailed balance* and reproduce the *equilibrium probability distribution* of the system.

A Monte-Carlo simulation essentially provides an implementation of such a transition function. For thermal systems one has to care about the last point from above, that is one needs to have an equilibration process before a high number s of *Monte-Carlo Steps* can be applied for the 'measurement'. The average is then taken over the configurations that occurred in these s steps. In thermal systems, one possible

realization of the algorithm to implement the Monte-Carlo step is the *Metropolis Algorithm*.

In the context of percolation theory however, we do not face most of the problems that come up for thermal systems, namely there is no equilibrium configuration, there is no critical slowing down and also there is no need for such requirements as ergodicity and detailed balance to be fulfilled. This implies that the implementation of the Monte-Carlo step in percolation theory can be rather simple: We go through the lattice, occupy each site with the given probability and do the same for the edges. This essentially constitutes one Monte Carlo step and is repeated a multiple number of times to produce a high number of independent lattice configurations. The expectation value of the observable that is to be investigated is computed by taking into account these configurations.

2.4 Some Results

In this section, after having reviewed some general features of phase transitions and also having pointed out the differences one encounters in the simulation of a percolative system as opposed to a thermal system, we will present some major results of percolation theory that are the basis for the further discussion of the present work. We will mostly deal with findings that hold for bond and site percolation theory, should the contrary be the case, we will give an explicit indication of this.

2.4.1 The Infinite Cluster

We now combine the graphical concept and the probability part introduced in Secs. 2.1.1 and 2.1.2 and ask what happens in the lattice if the probability p for a vertex to be occupied is changed. As already stated in the introductory example of Sec. 2.1.1,

it is intuitively clear that with an increase in the value of p the average cluster size will increase, since a higher value of p generally leads to a higher number of open edges. In a simple picture then, at some critical value p_c , a further small increase in p will allow large clusters to agglomerate and form a cluster C_{max} that spans the entire system, meaning that some vertex $y_b \in C_{max}$ in the bottom layer and some vertex $z_t \in C_{max}$ in the top layer are connected: $y_b \longleftrightarrow z_t$. Although in a finite system there exists a finite probability that the spanning cluster is not the biggest cluster in the system, this probability is very small and usually the percolating cluster can be identified with the cluster of maximal size, C_{max} . In the thermodynamic limit, where the lattice size $L \rightarrow \infty$, this would yield $|C_{max}| \rightarrow \infty$. Moreover, in a finite system, finite probabilities exist that more than one spanning cluster is present. In a finite system, we define the *infinite cluster*, C_∞ , by the following properties:

$$|C_\infty| = \max \{|C_i|\}, \quad (2.10)$$

and

$$y_b, z_t \in C_\infty, \quad (2.11)$$

where y_b and z_t have to fulfill the following requirements in a lattice of linear dimension L :

$$y_b = (i, j, \dots, 0), \quad (2.12)$$

$$z_t = (k, l, \dots, L), \quad (2.13)$$

if percolation is checked in the direction of the last coordinate.

The Percolation Probability

After having introduced the concept of an infinite cluster, we can define one principal quantity of interest: The *percolation probability*, also called *strength of the infinite*

cluster, $p_\infty(p)$ as the probability that a given vertex belongs to an infinite cluster,

$$p_\infty(p) = P_p(|C| = \infty). \quad (2.14)$$

This may also be written as

$$p_\infty(p) = 1 - \sum_{s=1}^{\infty-1} P_p(|c| = s), \quad (2.15)$$

since a given vertex either belongs to the infinite cluster or to some finite cluster.

The notation ' $\infty - 1$ ' as upper limit in the sum is meant to indicate that the infinite cluster is excluded in the summation. P_p can further be expressed as a sum over all existing cluster configurations, which are also called *lattice animals*, in the following way:

$$P_p(|c| = s) = \sum_{m,b} a_{smb} p^m q^b. \quad (2.16)$$

Here, a_{smb} is the number of lattice animals which are characterized by their number of vertices s , edges m and boundary edges b .

Intuitively it is clear that $p_\infty(p)$ is a monotonous function in p and has the limiting values $p_\infty(0) = 0$ and $p_\infty(1) = 1$. Furthermore, according to the above considerations, we expect a critical behavior of the percolation probability with a critical value, the *percolation threshold* p_c , yielding

$$p_\infty(p) = \begin{cases} = 0, & \text{if } p < p_c \\ > 0, & \text{if } p > p_c \end{cases}. \quad (2.17)$$

The percolation threshold is formally defined as

$$p_c = \sup\{p \mid p_\infty(p) = 0\}. \quad (2.18)$$

Uniqueness of the Infinite Cluster

As stated in the previous section, in a finite system, more than one percolating cluster can exist. For an infinite percolating system however, it can be proved that the infinite open cluster is unique, see [Gri99], where the following theorem is given:

Theorem 1 *If for some p it is $p_\infty(p) > 0$, then*

$$P_p(\exists \text{ exactly one infinite open cluster}) = 1.$$

For the proof, we may refer to the literature.

Continuity of the Percolation Probability

One will notice that in (2.17) the case $p = p_c$ has been left out. As stated in Ref. [Gri99], it is a known fact that for dimension $d = 2$ and for dimensions $d \geq 19$ there exists no infinite cluster right at the critical point: $p_\infty(p_c) = 0$. For dimensions $d \geq 3 \leq 19$ the situation is not clear. It is believed that $p_\infty(p_c) = 0$ for dimensions $d \geq 3$ also, but no rigorous results exist. On one hand this is, in a sense, required, since, as will be discussed in more detail later, an important conjecture of percolation theory is that $p_\infty(p)$ undergoes a second order phase transition at the percolation threshold p_c . It is thus required that $p_\infty(p)$ be continuous. The only way to fulfill this requirement on the whole interval $[0, 1]$ is to assign $p_\infty(p_c) = 0$. On the other hand, the existence of an infinite open cluster at the percolation threshold p_c , called *incipient infinite cluster* is discussed in this context, see for example [SA94]. However we will have to distinguish between our model, as an ideal, mathematical system that can be infinite in extent and the simulated physical system, which will always be finite and subject to errors of all kinds. In such a system it will be impossible to probe at exactly one value of the bond existence probability. Due to floating point representation imprecision and the system discreteness, we will always end up with an average taken over some small interval around the critical value p_c . We will thus deal with the subject in the following way: As long as we are considering ideal characteristics of our system, we will consider the percolation probability to be zero

right at the percolation threshold:

$$p_\infty(p_c) = 0, \quad (2.19)$$

which implies

$$p_c = \max\{p \mid p_\infty(p) = 0\}. \quad (2.20)$$

In the context of physical systems however, we shall abide by the imprecise notation of an infinite open cluster *at* the threshold, meaning the incipient cluster if probed in an interval around the critical value p_c , with the width given by the limitations of the numerical experiment.

The Critical Phenomenon

For percolation in one dimension, $d = 1$, there is no real critical phenomenon, as in a one-dimensional infinite system an infinite chain of occupied vertices is needed, which is only possible for a critical value $p_c^{d=1} = 1$, so that only one phase, the non-percolating one is accessible on a set with non-zero measure. The existence of a nontrivial critical phenomenon for dimensions $d \geq 2$ was shown by Broadbent and Hammersley, [BH57, Ham57, Ham59] as cited in [Gri89] with the following theorem¹.

Theorem 2 *If $d \geq 2$ then $0 < p_c^d < 1$.*

We can thus specify two phases of the process: A *subcritical phase* and a *supercritical phase*, where in the former we will almost ever only have finite open clusters, whereas in the latter there will be almost always an infinite open cluster present. The probability that there exists an open infinite cluster, $\psi(p)$, follows

$$\psi(p) = \begin{cases} 0, & \text{if } p < p_c \\ 1, & \text{if } p > p_c \end{cases}. \quad (2.21)$$

¹Again, we will not repeat the proof here, it can be found in the cited reference

This is only exactly true in the thermodynamic limit of an infinite system: $L \rightarrow \infty$. For finite L , finite-size-effects will 'smear out' the step function to some differentiable function. A more solid discussion of this effect is deferred to a later point, the phenomenon of finite-size effects and finite-size scaling will be discussed in Sec. 2.5.

Site versus Bond Percolation

In the site percolation model, introduced in 2.1.2, the definition of the percolation threshold is exactly the same as in the case of bond percolation, (2.18). However, if we perform a simulation on exactly the same lattice, what will be the numerical value of p_c^{site} , compared to p_c^{bond} ? It has to be noted, that a bond percolation model on a graph G may be reformulated as an equivalent site percolation model on a *covering graph* G_c , see [Gri99], for which

$$p_c^{bond}(G) = p_c^{site}(G_c). \quad (2.22)$$

For both processes on the same graph, however, we have

$$p_c^{bond}(G) \leq p_c^{site}(G). \quad (2.23)$$

On a high number of lattices, the strict inequality is true.

2.4.2 Cluster Size

Aside from the very important quantity, the percolation probability, another important property of percolation is the *mean cluster size*

$$\chi(p) = E_p(|C|). \quad (2.24)$$

It can, just as the percolation probability, be expressed in terms of the cluster size distribution, being the first moment, whereas the percolation probability represented

the zeroth moment:

$$\chi(p) = \sum_{s=1}^{\infty} s P_p(|C| = s), \quad (2.25)$$

where again $P_p(|C| = s)$ is the probability that a given vertex belongs to a cluster of size s . At this point a brief note concerning the difference between bond and site percolation is necessary. Basically, in site percolation a calculation of the mean cluster size is possible in exactly the same way: The question is, what the probability is, when going through the lattice and hitting *every* vertex with the same probability, that this arbitrarily chosen vertex is part of an s -cluster. Since in bond percolation every vertex is occupied, a distinction of open and closed vertices is not necessary. This is different in site percolation. When hitting every lattice site with equal probability, also closed vertices are included, which introduces an implicit dependence of the mean cluster size on the fraction of occupied sites, p . To avoid this influence, we have to introduce a normalization, the fraction of open sites. We thus generalize (2.25) to

$$\chi(p) = \frac{\sum_{s=1}^{\infty} s P_p(|C| = s)}{\sum_{s=1}^{\infty} P_p(|C|)}, \quad (2.26)$$

where

$$\sum_{s=1}^{\infty} P_p(|C|) = \begin{cases} 1 & \text{for bond percolation} \\ p & \text{for site percolation} \end{cases} \quad (2.27)$$

Also should we state that there is yet another way to define a mean cluster size. One can take the average over all clusters, which would be equivalent to asking what the mean cluster size is, if every *cluster* and not every site, as before, is hit with equal probability. Given the actual number of clusters with size s to be N_s , this amounts to defining the mean cluster size as

$$S = \frac{\sum_{s=1}^{\infty} s N_s}{\sum_{s=1}^{\infty} N_s}. \quad (2.28)$$

We will subsequently stick to the definition of the mean cluster size as given in (2.26) in the further discussion.

Although this is not a priori obvious, it is

$$\chi(p) < \infty \quad \text{if } p < p_c. \quad (2.29)$$

For values of p above the percolation threshold the sum in (2.25) diverges because of the existence of an infinite cluster:

$$\chi(p) = \infty \quad \text{if } p > p_c. \quad (2.30)$$

This can be remedied by introducing a truncated mean cluster size that does not take into account the infinite cluster:

$$\begin{aligned} \chi^f(p) &= E_p(|C|; |C| < \infty) \\ &= \sum_{s=1}^{\infty-1} s P_p(|C| = s). \end{aligned} \quad (2.31)$$

The symbolic notation ' $\infty - 1$ ' means that the infinite cluster is not included in the sum. If we consider $\chi^f(p)$ as a continuation of $\chi(p)$ on $p \in [p_c, 1]$, then $\chi(p)$ shows a singularity at $p = p_c$ and is finite on the rest of the interval $[0, 1]$. Whenever $p_\infty(p) = 0$, then $\chi(p) = \chi^f(p)$ naturally. The fact that both p_∞ and χ show a phase transition at the same one point p_c leads to calling percolation a model with a unique phase transition.

2.4.3 The Number of Open Clusters per Vertex

For completeness, we will just give a short definition of this quantity and come back to its postulated scaling behavior in Sec. 2.4.5. The Number of open clusters per vertex is defined in the following way:

$$\kappa(p) = \sum_{s=1}^{\infty} \frac{1}{s} P_p(|C| = s). \quad (2.32)$$

The first terms can be calculated using elementary considerations for the probabilities of clusters of a given size and then summing over the cluster size. The number of open clusters per vertex is also referred to as f-function.

2.4.4 Cluster Numbers

In this section we will present a short discussion about cluster numbers in percolation systems. At some points, however, when the possibility arises in a natural way, we will also wander off to other quantities, always giving reference though to the section where we first introduced it or where we will give a more precise discussion. Also do we have to clarify that by *cluster numbers* we do not mean the total number of open clusters per vertex, but rather the number of open clusters of a given size s per vertex, that is, the cluster size distribution. For the sake of simplicity we will mostly argue on the basis of site percolation, which does not give a restriction on the general results.

In the previous section we have already argued with the different moments of the cluster size distribution $P_p(|C| = s)$. It has to be noted, however, that this term is somewhat imprecise. $P_p(|C| = s)$ represents the probability that an arbitrary site (every site in the lattice is hit with equal probability) belongs to a cluster with s sites. The real cluster numbers shall be denoted by n_s , by which we mean the actual number of clusters of size s , N_s , normalized by the number of sites in the lattice N :

$$n_s = \frac{N_s}{N}. \quad (2.33)$$

Then, the probability that a given vertex belongs to an s -cluster, is given by the product of n_s with the actual cluster size s :

$$P_p(|C| = s) = n_s(p) s. \quad (2.34)$$

For a calculation of n_s it is necessary to know the number of different configurations clusters can be realized in with exactly s sites, which we denote by g_{st} , compare (2.16). In (2.16) we already introduced the corresponding quantity a_{smb} for bond percolation. Here, we have one index less, s being the number of vertices in the cluster and t being

the number of *perimeter* vertices, which is the number of all empty neighbor vertices, including internal unoccupied, neighboring vertices. To get n_s , we then have to sum over all of these configurations, multiplied with their respective statistical weight. For a configuration with s vertices and t perimeter sites, this is just $p^s(1-p)^t$, giving as the number of size s clusters:

$$n_s = \sum_t g_{st} p^s (1-p)^t. \quad (2.35)$$

One-dimensional exact Solution

In percolation we deal with statistically independent events. Thus, we have factorizing probabilities always. Therefore, the probability to have s sites occupied is p^s . For these occupied sites to be a cluster we furthermore need one unoccupied site at each end of such a linear configuration of occupied sites. The probability to have this condition fulfilled is simply given by $(1-p)^2$. Neglecting chain end effects, every site has probability $p^s (1-p)^2$ of being, say, the right end of the linear cluster and with L sites in the whole lattice the total number of s clusters is $L p^s (1-p)^2$, giving a normalized number of s -clusters per vertex

$$n_s(p) = p^s (1-p)^2. \quad (2.36)$$

The percolation threshold in a one-dimensional system does not allow for a real phase transition behavior: In a lattice of L sites, there will be

$$(1-p) L \xrightarrow{L \rightarrow \infty} \infty$$

empty sites in the linear chain, leading to a critical value of

$$p_c = 1. \quad (2.37)$$

Defining the probability for an occupied site chosen at random, to belong to an s -cluster as

$$w_s = \frac{n_s s}{\sum n_s s},$$

we can calculate the mean cluster size as, cf. (2.26)

$$\begin{aligned} \chi &= \sum w_s s \\ &= \sum \frac{n_s s^2}{\sum n_s s}. \end{aligned} \quad (2.38)$$

This equation still represents a general result. The denominator is equal to p and after evaluating the sum in the numerator, by turning it into derivatives of easier sums, this gives

$$\chi(p) = \frac{1+p}{1-p} \quad \text{for } p < p_c. \quad (2.39)$$

With $p_c = 1$, we thus encounter a divergence in the mean cluster size for $p \rightarrow p_c$, which will also turn out to be the case in higher dimensions. In one dimension it is also easy to calculate the correlation function and the correlation length, which we introduced in the realm of the general discussion of phase transitions in (2.3). The probability that a site at some position x is in the same cluster as the site at the origin requires the x connecting sites to be occupied, which happens with probability p^x . This is already the correlation function which we just rewrite in an exponential form

$$g(x) = \exp\left(\frac{-x}{\xi}\right), \quad (2.40)$$

thus defining the correlation length ξ as

$$\xi = -\frac{1}{\ln(p)}. \quad (2.41)$$

For $p \approx p_c = 1$ the logarithm can be expanded as $\ln(1 - x) \approx -x$ for $x \ll 1$, which gives

$$\xi = \frac{1}{p_c - p}. \quad (2.42)$$

Thus also the correlation length diverges at the threshold with a critical exponent, see Table 2.1,

$$\nu = -1. \quad (2.43)$$

The Cayley Tree

The second exactly solvable lattice is the so called Bethe lattice or Cayley tree, which we already introduced in Sec. 2.1.5. If we try to find a way connecting the origin to the surface, then we find $(z - 1)$ new sites on which we can continue at every branching, $p(z - 1)$ of which will be occupied on average. We need at least one site occupied at every branching for a continuous path to exist and thus:

$$p_c = \frac{1}{z - 1}. \quad (2.44)$$

Since we can, without any argumentative change, replace site by bond in the above considerations, (2.44) is valid for both site and bond percolation. If we now want to calculate n_s , we can use (2.35). It turns out that in the Bethe lattice the number of perimeter sites is uniquely related to the number of sites s in the cluster, thus g_{st} reduces to g_s . The relation of perimeter sites t to s reads

$$t = 2 + s(z - 2), \quad (2.45)$$

as a single site has 2 empty neighbors, two sites have $(z - 2)$ neighbors and every site more adds another $(z - 2)$ empty neighbors. Without explicitly deriving g_s we can then calculate the ratio $n_s(p)/n_s(p_c)$:

$$\frac{n_s(p)}{n_s(p_c)} = \left(\frac{p}{p_c}\right)^s \left(\frac{1-p}{1-p_c}\right)^{2+s(z-2)}. \quad (2.46)$$

For the sake of simplicity we will set $z = 3$ in the further derivation and do the following (exact) expansion:

$$\begin{aligned}
f(p) &= \frac{p}{p_c} \left(\frac{1-p}{1-p_c} \right) \\
&= f(p_c) + f'(p_c)(p-p_c) + \frac{1}{2} f''(p_c)(p-p_c)^2 \\
&= 1 + \frac{1-2p_c}{p_c(1-p_c)}(p-p_c) - \frac{1}{p_c(1-p_c)}(p-p_c)^2 \\
&= 1 - 4(p-p_c)^2,
\end{aligned}$$

where in the last equality we have made use again of the fact that we set $z = 3$ finally arriving at

$$\begin{aligned}
p_c &= \frac{1}{z-1} \\
&= \frac{1}{2}
\end{aligned}$$

Plugging this result back into (2.46) we have

$$\frac{n_s(p)}{n_s(p_c)} = \left(\frac{1-p}{1-p_c} \right)^2 (1 - 4(p-p_c)^2)^s \tag{2.47}$$

$$\propto \exp(-c s) \tag{2.48}$$

where

$$c = -\ln(1 - a(p-p_c)^2) \tag{2.49}$$

$$= a(p-p_c)^2 + \mathcal{O}((p-p_c)^3), \tag{2.50}$$

which is true for $1 - a(p-p_c)^2 \ll 1$. Making use of the heuristic argument that the mean cluster size χ (second moment of the cluster size distribution) has to diverge at the threshold p_c , which, with (2.38), is not possible for an exponential decay of n_s , we conjecture the plausible form

$$n_s(p_c) \propto s^{-\tau}, \tag{2.51}$$

for large s . This defines the so-called Fisher-exponent τ . By calculation of χ and comparison with the general form for χ (not derived here, see, e.g. [SA94]),

$$\chi \propto \frac{1}{p - p_c}, \quad (2.52)$$

we have

$$\tau = 5/2. \quad (2.53)$$

Thus finally we arrive, with (2.46), at

$$n_s(p) \propto s^{-5/2} \exp(-c s), \quad (2.54)$$

valid for large s .

To conclude this section, we want to point out why the Bethe lattice solution is useful as an approximation of high-dimensional lattices. For 'normal' lattices we have for the relation of surface of some volume to the volume itself

$$\partial V \propto V^{1-1/d}. \quad (2.55)$$

In the Bethe lattice with a branching factor z , a cluster that has branched t times will have

$$\begin{aligned} N_t &= 1 + z \sum_{n=0}^{t-1} (z-1)^n \\ &= \frac{z(z-1)^t - 2}{z-2} \end{aligned} \quad (2.56)$$

sites in the cluster of which

$$S_t = z(z-1)^{t-1} \quad (2.57)$$

sites are surface sites. This gives the ratio

$$\begin{aligned} \frac{S_t}{N_t} &= \frac{z(z-1)^{t-1}(z-2)}{z(z-1)^t - 2} \\ &\stackrel{t \gg 1}{\approx} \frac{(z-2)}{(z-1)}. \end{aligned} \quad (2.58)$$

I represents a finite limit. In normal lattices, this is only attained, as (2.55) shows, for a dimension $1/d = 0$. Thus, percolation on a Cayley tree should approximatively describe percolation on non-loop-free lattices for higher dimensions $d \rightarrow \infty$. In practice, the results derived for the Bethe lattice hold for dimensions $d > 6$.

Conjectured Scaling Behavior of n_s

For general lattices and dimensions, no exact solution for the cluster numbers is known. Aside from the method of *series expansion*, where the cluster numbers for clusters with a small number of vertices are calculated exactly and then extrapolation methods for $s \rightarrow \infty$ are employed, one will thus have to rely on conjectures and checking them in numerical experiments. We might, with the derivations of the previous section, try to postulate a general formula for the cluster numbers. It would be very natural to assume

$$n_s \propto s^{-\tau} \exp(-c s). \quad (2.59)$$

This is essentially the solution for the Cayley tree, but here, we will allow a general exponent for c :

$$c \propto |p - p_c|^{1/\sigma} \quad \text{for } p \rightarrow p_c. \quad (2.60)$$

An obvious problem with this form is the fact that the one-dimensional solution is not contained as special case, since, using $\exp(\ln p) \approx \exp(p - 1)$ for $p \approx p_c$, the one-dimensional result (2.36) can be cast into

$$n_s = (p_c - p)^2 \exp(-(p_c - p)s), \quad (2.61)$$

which does not reproduce the power law in terms of s . A second problem arises with respect to possible divergences in the cluster number. According to (2.35) the cluster number is a finite polynomial in p , and hence n_s and $\frac{d^n n_s}{dp^n}$ for all n should stay finite.

However, with (2.60), this is not the case for non-integer values of $1/\sigma$. Thus, we take $z' = cs \propto |(p - p_c)|^{1/\sigma} s$ to the power of σ as new z :

$$z = (p - p_c) s^\sigma. \quad (2.62)$$

In the postulate above, (2.47), the assumption for the ratio $n_s(p)/n_s(p_c)$ is an exponential behavior,

$$\frac{n_s(p)}{n_s(p_c)} \propto \exp(z).$$

For a more general scaling assumption which should also reproduce the one-dimensional result, the conjecture should just read

$$\frac{n_s(p)}{n_s(p_c)} = f(z). \quad (2.63)$$

We then have for the cluster numbers, with $n_s(p_c)$ from (2.51),

$$n_s(p) = s^{-\tau} f((p - p_c)s^\sigma) \quad \text{for } p \rightarrow p_c, s \rightarrow \infty. \quad (2.64)$$

The exact form of $f(z)$ has to be determined in simulations. A problem that occurred for the first scaling hypothesis (2.59) has now been remedied: With the assumption that $f(z)$ analytical everywhere, n_s will show no singularities, as expected.

The one-dimensional case now is included with $\sigma = 1$ and $\tau = -2$, compare (2.61):

$$n_s = s^{-2} z^2 \exp(z).$$

2.4.5 Scaling Theory

We already applied ideas of scaling theory in the previous section with the scaling assumption (2.64) for the cluster numbers. Scaling theory makes predictions about the behavior of macroscopic observables for p in the vicinity of the critical value p_c . The basis of scaling theory has not yet been proven in a strict mathematical sense,

[Gri99], but the conjectures have been verified to a very good extent in simulations. We will, in the following, derive two *scaling laws*, but deprive us of a derivation of the remaining scaling laws, but instead summarize the general idea of scaling theory.

Percolation Probability

With the new notation for cluster numbers introduced in the previous section, (2.34), we have for the percolation probability in site percolation, in analogy to (2.15) for bond percolation,

$$p_\infty(p) = p - \sum_{s=1}^{\infty-1} n_s(p)s. \quad (2.65)$$

At the critical point, it is $p_\infty = 0$ and thus we can add and subtract p_c in the following form:

$$\begin{aligned} p_\infty &= (p - p_c) + \sum_{s=1}^{\infty-1} n_s(p_c)s - \sum_{s=1}^{\infty-1} n_s(p)s \\ &= (p - p_c) + \sum_{s=1}^{\infty-1} (n_s(p_c) - n_s(p))s \end{aligned} \quad (2.66)$$

where for the convergence of the first sum, $\tau > 2$ is necessary. Although $f(z)$ does not have to follow an exponential decay according to the new scaling assumption (2.63), it will in any case show a decay. This, together with the fact that for the Bethe lattice we found an exponential decay, is a heuristic motivation that only large cluster numbers essentially contribute in the sum, which allows for replacing the sum

by an integral,

$$\begin{aligned}
p_\infty &= \int ds \, s^{1-\tau} (f(0) - f(z)) \\
&= \int dz \, \frac{1}{\sigma(p - p_c)} s^{2-\sigma-\tau} (f(0) - f(z)) \\
&= |(p - p_c)|^{(t-2)/\sigma} \int \frac{dz}{\sigma} |z|^{-1-(\tau-2)/\sigma} (f(0) - f(z)) \\
&\propto |(p - p_c)|^\beta.
\end{aligned} \tag{2.67}$$

This introduces the critical exponent β

$$\beta = \frac{\tau - 2}{\sigma}. \tag{2.68}$$

The limits of the integral are now case dependent: 0 to $+\infty$ for $p > p_c$ and $-\infty$ to 0 for $p < p_c$, which is why the absolute values are introduced. We have furthermore used

$$ds = \frac{1}{\sigma(p - p_c)} s^{1-\sigma} dz, \tag{2.69}$$

$$s = z^{1/\sigma} (p - p_c)^{-1/\sigma}, \tag{2.70}$$

in the derivation. For negative values of z , the factor of proportionality in the last equation of (2.67) has to vanish, that is the integral should be zero:

$$\int dz \, |z|^{-1-\beta} (f(0) - f(z)) = 0.$$

This brings up a requirement to be fulfilled by $f(z)$.

Mean Cluster Size

An analogous calculation for the second moment of the cluster size distribution χ yields another scaling law. It is, see (2.26),

$$\begin{aligned}
 \chi &\propto \sum s^2 n_s \\
 &\propto \int ds s^{\tau-2} f(z) \\
 &= |p - p_c|^{(\tau-3)/\sigma} \int \frac{dz}{\sigma} |z|^{(3-\tau)/\sigma-1} f(z) \\
 &\propto |p - p_c|^{-\gamma}, \tag{2.71}
 \end{aligned}$$

which introduces another critical exponent,

$$\gamma = \frac{3 - \tau}{\sigma}. \tag{2.72}$$

Equations like (2.68) and (2.72) are known as *scaling laws* and they put up relations between the different critical exponents for different macroscopic observables.

The Correlation Length

We can introduce a probability $\tau_p^f(y, z)$ that for a given vertex y in a cluster C also some other vertex $z = (n, 0, 0, \dots)$, lying directly 'above' y belongs to the same finite open cluster. It is conjectured that τ_p^f follows

$$\tau_p^f(y, z) \approx \begin{cases} n^{2-d-\eta}, & \text{if } p = p_c \\ \exp(-n/\xi(p)), & \text{if } p \neq 0, p_c, 1 \end{cases}. \tag{2.73}$$

Here, d is the dimension, η is yet another critical exponent and $\xi(p)$ is the correlation length. For p near to p_c the behavior of $\xi(p)$ has the form

$$\xi(p) \approx |p - p_c|^{-\nu}, \tag{2.74}$$

a behavior which we already found with $\nu = 1$ in the one dimensional example, see (2.41). The notation ' \approx ' signifies that ξ and $|p - p_c|$ satisfy

$$\lim_{p \searrow p_c} \frac{\log \xi(p)}{\log |p - p_c|} = -\nu. \quad (2.75)$$

Scaling Theory

In a brief summary, the basic ideas of scaling theory are as follows. Macroscopic quantities behave as powers of $|p - p_c|$ in the vicinity of the critical point p_c . Examples are the correlation length ξ , the percolation probability p_∞ and the mean cluster size χ . The correlation length gives a length scale for the system under observation, one interpretation is to see it as the minimal length scale on which percolation at p can be distinguished from percolation at p_c . The correlation length diverges when the system approaches the critical point. A further result of scaling theory are the scaling laws, which the critical exponents are conjectured to satisfy and which reduce the set of seven critical exponents to a set of two independent exponents. A further assumption is that the critical exponents satisfy the *hyperscaling relations*, which involve the critical exponents and the dimension d of the system. The hyperscaling relations are only valid however for $d \leq 6$. As already discussed for phase transitions in general, the critical exponents are universal, depending only on the dimension of the system, not the microscopic structure. A heuristic justification takes as argument that at the critical point, where the critical exponents determine the behavior of the macroscopic observables, the correlation length diverges, which makes any information on the microscopic structure of the system irrelevant. Related to that is the fact that at the critical point, the infinite cluster is fractal with a fractal dimension $D = 91/48 \simeq 1.89$ for site percolation on two-dimensional lattices, see [Fed88]. This so called *incipient infinite cluster* is self-similar on all length-scales.

2.4.6 Analogies of Percolative Phase Transitions to Thermal Phase Transitions

Before, in the next section, we proceed to a discussion of Finite Size Scaling we want to show the existing analogies between the quantities introduced above for percolation theory and the thermal functions discussed in the realm of thermal phase transitions in Sec. 2.2. We do so in the concise form of Table 2.2. In Table 2.3 we give a reference

Percolative Function	Notation	Thermal Function	Notation
Distance from critical point	$p - p_c$	Distance from critical point	$T - T_c$
F-Function	$\kappa(p)$	Free Energy	F
Percolation Probability	$p_\infty(p)$	Spontaneous Magnetization	M
Mean Cluster Size	$\chi(p)$	Susceptibility	χ
Correlation Length	ξ	Correlation Length	ξ

Table 2.2: Percolative functions and their analogous counterpart in thermal systems.

to the section in which we introduced or discussed the respective percolative function.

Percolative Function	Sec.
Number of Open Clusters per vertex	2.4.3
Percolation Probability	2.4.1
Mean Cluster Size	2.4.4, 2.4.5
Correlation length	2.2.3, 2.5, 2.4.5

Table 2.3: Percolative functions and the section in which they were first introduced or further discussed.

2.5 Finite Size Scaling

Let us consider a finite, d -dimensional site percolation system with occupation probability p . As soon as we have $p > 0$ in this finite system, there is a non-zero probability

that *every* site in the system will be occupied, given by

$$(p^L)^d = \exp(L^d \ln p). \quad (2.76)$$

This would not be possible in an infinite system and is an indication that the behavior qualitatively changes in a finite system with respect to the infinite one. In a finite lattice the singularities associated with the critical behavior will be smoothed out. In simulations, it is found that the conjectured power laws in $|p - p_c|$ still hold, but with a shifted value of p_c . How does the shifted value $p_c(L)$ approach the real value $p_c = p_c(\infty)$? Let us consider the one-dimensional example again. We call the probability that there exist a spanning cluster Π . It is given by

$$\begin{aligned} \Pi &= p^L \\ &= \exp(-L/\xi), \end{aligned} \quad (2.77)$$

thus defining the correlation length ξ as

$$\xi(p) = -\frac{1}{\ln p}, \quad (2.78)$$

like in (2.41). In an infinite system, we would expect Π to show a step-function like behavior, with $\Pi = 1$ at $p = p_c = 1$ and $\Pi = 0$ for $p < p_c$. According to our above consideration, there will be a smoothed behavior present for $L < \infty$. We may then define an effective threshold, at a p defined by a more or less arbitrary value of Π . We choose to define the effective threshold in the following way:

$$p_{eff} = \Pi^{-1}\left(\frac{1}{e}\right). \quad (2.79)$$

With the expansion

$$-\frac{1}{\ln p} \approx \frac{1}{1-p}, \quad (2.80)$$

valid for $p \approx 1$, we have for the effective threshold, as $\Pi \stackrel{!}{=} 1/e$, implying $L = \xi$,

$$p_{eff} = 1 - \frac{1}{L}. \quad (2.81)$$

Thus the effective threshold at a linear dimension L approaches the true threshold in an infinite system as

$$p_c - p_{eff} = L^{-1/\nu}, \quad (2.82)$$

with

$$\nu = 1. \quad (2.83)$$

We now want to apply the same concept to higher dimensions. Although the situation is not as easy as in one dimension, we conjecture an essentially similar, but generalized behavior. With Π again being the spanning probability, we postulate the following scaling behavior for Π in finite systems:

$$\Pi(p, L) = g((p - p_c)L^{1/\nu}) \quad \text{for} \quad |p - p_c| \ll 1, \quad L \gg 1. \quad (2.84)$$

Then the derivative of Π with respect to p , which gives the probability that the system starts percolating if p is increased by dp , reads

$$\frac{d\Pi}{dp} = \frac{dg}{dz} L^{1/\nu}. \quad (2.85)$$

Here now we take the effective threshold to be the average threshold at which, averaged over $p \in [0, 1]$, the system starts percolating:

$$\begin{aligned} p_{eff} &= p_{av} \\ &= \int_0^1 dp \, p \frac{d\Pi}{dp}. \end{aligned} \quad (2.86)$$

This can be rewritten in terms of $z = (p - p_c)L^{1/\nu}$, yielding

$$\begin{aligned}
p_{eff} &= \int_0^1 dp \, p \frac{dg}{dz} L^{1/\nu} \\
&= \int_{z(p=0)}^{z(p=1)} dz \, \frac{dg}{dz} (zL^{-1/\nu} + p_c) \\
&= L^{-1/\nu} \int_{z(p=0)}^{z(p=1)} dz \, z \frac{dg}{dz} + p_c \int_{z(p=0)}^{z(p=1)} dz \, \frac{dg}{dz}. \tag{2.87}
\end{aligned}$$

Since we have

$$\begin{aligned}
\int_{z(p=0)}^{z(p=1)} dz \, \frac{dg}{dz} &= \int_0^1 dp \, \frac{d\Pi}{dp} \\
&= \Pi(1) - \Pi(0) \\
&= 1, \tag{2.88}
\end{aligned}$$

we deduce that the effective threshold approaches the real threshold as

$$\begin{aligned}
p_{eff} - p_c &= L^{-1/\nu} \int_{z(p=0)}^{z(p=1)} dz \, z \frac{dg}{dz} \\
&\propto L^{-1/\nu} \quad \text{for } |p_{eff} - p_c| \ll 1, \, L \ll 1. \tag{2.89}
\end{aligned}$$

As this finite size scaling is only valid for large lattice sizes, in the application systematic errors will occur. In higher dimensions no estimate for these deviations exists, we will come back to the question of the systematic errors at a later point, see Sec. 3.7. In the definition of the effective threshold (2.86), it is not at all necessary to define the effective threshold as the average threshold, as we have done. It would be equally

possible to choose the inflexion point of Π , or, as we have done in the discussion for one dimension, to set $p_{eff} = \Pi^{-1}(p')$, where p' can be some value in the smoothed transition region of Π . The result for how this effective threshold approaches the real one, (2.89), does still hold.

2.6 Percolation in Nuclear Physics

Percolation has been introduced in nuclear physics by Bauer to propose a model of fragmentation reactions, see [BDMP85, BPDM86, BBDG87, Bau88, Baud]. We will briefly present the essential features of this model, called the nuclear lattice model. Although this is, by no means, a restriction of the model, we just consider fragmentation reactions of the type

$$p + A_T = A_F + X. \quad (2.90)$$

As underlying lattice the simple cubic lattice is chosen and sites on this lattice are populated in an approximately spherical way to model the target nucleus. Deformed nuclei could also be considered, but the results are not changed essentially. Thus the lattice sites model the nucleons of the target nucleus and at the initial state each nucleon is connected by bonds to its six nearest neighbors. An impact parameter b is chosen and according to the so-called fireball geometry the nucleons in the cylindrical fireball channel, that is, the participants, are removed from the lattice. However, as stated in [BPDM86], since mostly only 6 – 8 nucleons are removed, the effect is not very important and basically the same results are obtained for a simulation that does not take care of the fireball scenario. This has the further implication that also the impact parameter b does not have a big influence on the results.

In this model, the breaking probability

$$p_b = (1 - p) \quad (2.91)$$

is chosen as input parameter, where p , as before, denotes what we called the bond existence probability. Using Monte Carlo techniques, a computer simulation is performed in which nearest neighbor bonds are broken according to p_b . In the basic version of this model, spin and isospin degeneracy are assumed, so that it suffices to have one bond breaking probability p_b . In the next step, cluster counting is performed and the cluster size is recorded. In the simulation it is then integrated over the impact parameter b , with the mass and multiplicity distribution for one value of p_b as result. Assumptions made for the realization of this model are as follows. The motion of the nucleons in the target nucleus can be neglected, which amounts to saying that the projectile sees a frozen image of the target, which is approximately valid in the region treated with the model, where the proton energy lies far above the Fermi energy of the target nucleons. As a further point, no energy conservation is present in the model. It seems however, that, since the proton energy is sufficient to completely fragment the target, energy conservation is not an important factor in the determination of the mass spectra. A physical interpretation of the breaking probability is possible through an analogy with the Ising model of ferromagnets. It is possible, as cited in [BPDM86], to show that the breaking probability is related to temperature in the following way:

$$p_b = \exp(-E_b(T)/T), \quad (2.92)$$

where for real nuclei at low temperatures

$$E_b(t) = 8 - \frac{1}{8}T^2. \quad (2.93)$$

The simulation data reproduces the mass yield curves and multiplicity distributions found in nuclear experiment of proton induced Multi-Fragmentation very well.

The fact that in the basic version of the model only one bond breaking probability was used is no inherent restriction of the model and extensions of it have been inves-

tigated, [Baud], using site-bond percolation with two components and two different bond breaking probabilities. This system, in which one can model varied isospin asymmetries, showed the same phase transition behavior as a one-component bond percolation model with isospin symmetry. Further details about a two-component percolation model will be discussed in Chapter 3.

Chapter 3

Two-Component Site-Bond Percolation

After reviewing the underlying ideas of percolation and phase transitions in general in Chapter 2, we want to focus on one special percolation model, that is percolation with two components on a simple cubic lattice using the combined site-bond percolation approach. Some aspects of this model were investigated by us in the framework of this thesis' research and we will present the results thereof in the following sections.

3.1 General Case: N Components

Let us begin with a description of the model we have used in the most general formulation. Although later on, we will consider a graph of dimension $d = 3$ in the special case of the structure of a simple cubic lattice, we don't make any assumptions about the lattice dimension or the lattice structure in this general section. The approach that is presented here is completely free of all such restrictions.

Thus we have a lattice of dimension d , as described in 2.1.1, and we have N different components with which the vertices are populated. Then there exist

$$A_{bp} = \binom{N + 2 - 1}{2} \quad (3.1)$$

different bond existence probabilities, one for each possible combination of sites to be connected. The bonds are assumed to be directionless, meaning that the probability of an edge to be open does only depend on the state of the two vertices it is connecting, not on their respective localization. There is another set of free parameters associated with the concentrations of the different species that populate the lattice. These are the component fractions

$$f_i = \frac{N_i}{\sum_{i=1}^N N_i}, \quad (3.2)$$

where the N_i 's are the actual number of particles of component i . Naturally, the component concentrations f_i have to satisfy

$$\sum_{i=1}^N f_i = 1. \quad (3.3)$$

Because of the normalization condition, the component concentrations constitute $(N - 1)$ free parameters. Overall we then have

$$A_{par} = (N - 1) + \binom{N + 2 - 1}{2} \quad (3.4)$$

free parameters a_i to vary.

The main question we are pursuing is at which parameter regime $\{a_i^{inf}\}$ in the A_{par} -dimensional parameter space an infinite network C_∞ of connected vertices is present in the lattice, that is, at which region $\{b_i^{inf}\}$ the percolation probability $p_\infty(\{a_i\})$ is nonzero:

$$\{b_i^{inf}\} = \{a_i : p_\infty(a_i) \neq 0\}, \quad (3.5)$$

and, more specific, where and in which form, the percolation probability changes from zero to a finite value. The particular type of bond shall be irrelevant for it to belong to the infinite cluster. Although there exists no principle argument against this approach, it is quite impractical for a system with $N \geq 3$. It would be highly

desirable to be able to reduce the dimensionality of the parameter space. Ideally one would hope for a reduction of the dependence of the order parameter, p_∞ in this case, on one variable at fixed component concentrations. We propose one such variable in following the definitions of [Baued], generalizing them to N components. In analogy to the bond existence probability in ordinary bond percolation processes, which gives the density of bonds present in the system under observation, we introduce the scaled control parameter p_+ ,

$$p_+ = \sum_{i \geq j=1}^N \alpha_{ij} p_{ij}. \quad (3.6)$$

Here, the p_{ij} 's denote the bond existence probability on an edge that has endvertices occupied by species i and j . The α_{ij} 's give the probability to find a nearest neighbor edge that connects two sites of flavors i and j :

$$\begin{aligned} \alpha_{ij} &= 2f_i f_j \\ &= \alpha_{ji}. \end{aligned} \quad (3.7)$$

Also the α_{ij} 's are normalized and thus subjected to the constraint

$$\sum_{i \geq j=1}^N \alpha_{ij} = 1. \quad (3.8)$$

This should provide the essential tool for a simulation aimed at answering the question related to (3.5) and we will present results in Sec. 3.2.

3.2 Two Components using the Natural Variables

We do not want to go into the detail of the simulation techniques used, at this point, but merely present the results, deferring a deeper discussion of the simulation techniques to Sec. 3.3. In Appendix A we show the source code of the programs

used in the simulations. We have performed simulations on 16^3 , 32^3 , 64^3 and 128^3 simple cubic lattices and set $N = 2$, the latter having as only argument the ease of visualization of the results, which would hardly be possible for $N > 2$. However, as there exists no fundamental constraints by setting $N = 2$, the results shown in this section should also hold for $N > 2$.

3.2.1 General Considerations

For simplicity we shall call one species *blue*, the other *red*. With $N = 2$ we have as number of free parameters

$$A_{par} = 4, \quad (3.9)$$

which are the fraction of one component, say of the blue sites, f_b , and three bond existence probabilities: p_{bb} for bonds connecting two blue sites, p_{rr} for bonds with two red endvertices and p_{\neq} for *b-r*-bonds. We will set

$$p_{=} \equiv p_{bb} = p_{rr}, \quad (3.10)$$

thus introducing a symmetry in the system. This can be motivated by, for example, considerations like isospin symmetry, where the e^+e^+ and e^-e^- interactions are identical. We furthermore have

$$p_{\neq} = p_{br} \quad (3.11)$$

$$= (1 - p_{=}). \quad (3.12)$$

Given these conditions, (3.6) now reads

$$p_+ = \alpha_{=}p_{=} + \alpha_{\neq}p_{\neq}, \quad (3.13)$$

where (3.7) has become

$$\begin{aligned}\alpha_{\neq} &= 2f_b(1 - f_b) \\ &= \frac{1}{2} - 2\left(f_b - \frac{1}{2}\right)^2\end{aligned}\quad (3.14)$$

$$\begin{aligned}\alpha_{=} &= f_b^2 + (1 - f_b)^2 \\ &= \frac{1}{2} + 2\left(f_b - \frac{1}{2}\right)^2.\end{aligned}\quad (3.15)$$

Here we have replaced the double index by a more intuitive notation for just two components. Due to the normalization condition (3.8) we have

$$\alpha_{=} = (1 - \alpha_{\neq}). \quad (3.16)$$

We carry out simulations according to these principles and with the techniques as described in Sec. 3.3

3.2.2 Simulation Results

In Fig. 3.1 we show the results of the simulations, namely p_{∞} as a function of the two control parameters $p_{=}$ and p_{\neq} . We see that the percolation probability p_{∞}

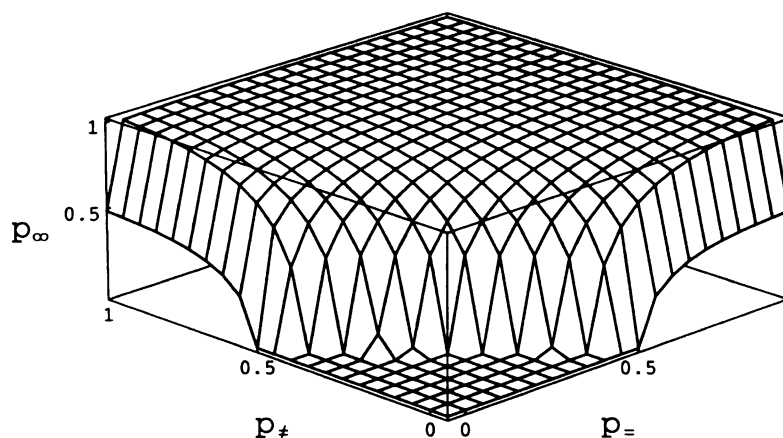


Figure 3.1: Probability to belong to the infinite cluster, p_{∞} , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_{=}$ and p_{\neq} , calculated for a fraction of the blue species of $f_b = 0.5$.

changes from 0 (front corner) to 1 (back corner) for $p_{=} \rightarrow 1$ and $p_{\neq} \rightarrow 1$, with a critical line of a second order phase transition in the $(p_{=}, p_{\neq})$ -plane. We expect some parametric dependence on the concentration of one of the two species. We chose to take f_b , also possible would be the concentration of the red species in the lattice, f_r . In Fig. 3.1 we have set $f_b = 0.5$. We show the effect of varied f_b in Figs. 3.2 and 3.3, where $f_b = 0.2$ and $f_b = 0.0$ respectively. It can be seen that, according to

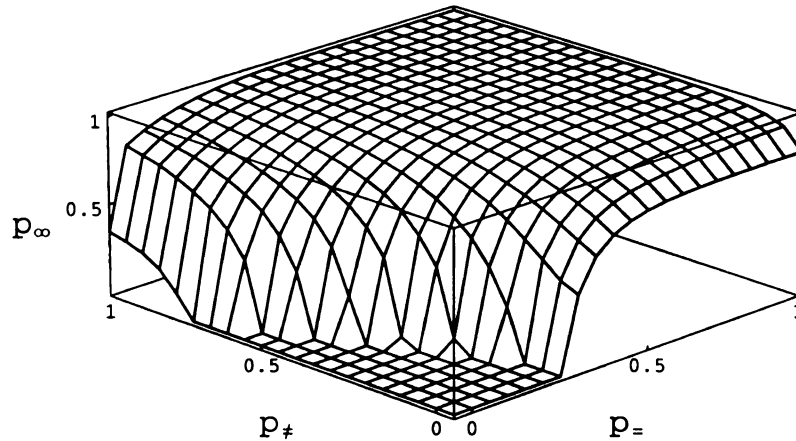


Figure 3.2: Probability to belong to the infinite cluster, p_{∞} , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_{=}$ and p_{\neq} , calculated for a fraction of the blue species of $f_b = 0.2$.

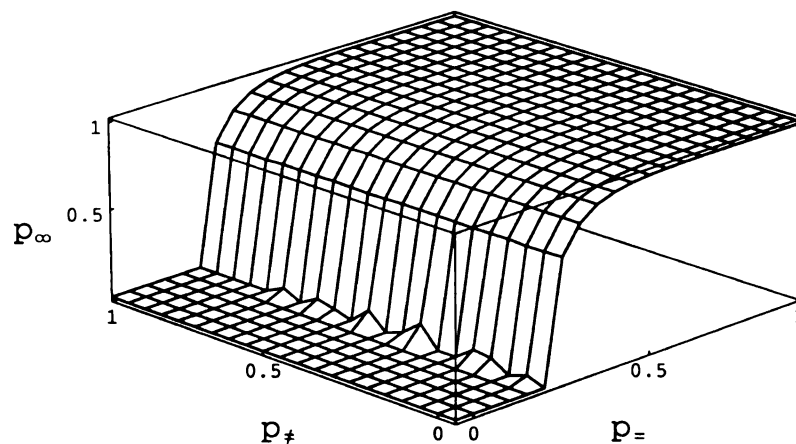


Figure 3.3: Probability to belong to the infinite cluster, p_{∞} , in a simple cubic two-component site-bond percolation lattice of size 128^3 as a function of the two parameters $p_{=}$ and p_{\neq} , calculated for a fraction of the blue species of $f_b = 0.0$.

the expectations, for only one component populating the lattice, $f_b = 0$ or $f_b = 1$, we regain a two-dimensional curve which seems to scale, at least on an eye-analysis basis, as predicted by scaling theory, compare Sec. 2.4.5 and in particular (2.67). Before, in Sec. 3.4, we will come to a realization of the ideas presented in our general discussion in Sec. 3.2.1, we will explain in more depth the simulation techniques used, in Sec. 3.3.

3.3 Simulation Techniques

The simulation programs are coded in **FORTRAN** and the source code can be found in Appendix A. Several programs have been written to accommodate different needs. First, there is a general program, which determines the percolation probability p_∞ , the probability that a spanning cluster exists, ψ , and the number of open clusters per vertex. Three other programs have been written, aimed at more specific tasks, two to determine the critical value of p_+ through the critical values of $p_ =$, $p_ \neq$, respectively, and one to find the threshold of f_b . In the following sections, we will, in a concise manner, describe the main features of the simulation as implemented in the programs.

3.3.1 General Features

We aim at simulating a simple cubic lattice of dimension n^3 , with a maximum lattice size $maxn^3$. The implementation has been realized as a three dimensional logical array `neutron(maxn,maxn,maxn)` in **FORTRAN**. Using a (pseudo) random number generator taken from [PTVF92], modified to work with double precision, we sweep through the lattice in order to determine which site is occupied by which of the two possible species. In the source code, the notation is `neutron(i,j,k)`, meaning in a more neutral formulation the blue components. As already stated in Sec. 2.3, a Monte Carlo step in the case of percolation just consists of generating one particular configuration

of the lattice. We do so by generating a pseudo random number `ran` at every vertex $\vec{y} = (i, j, k)$ and then comparing it to the probability of having a blue site, f_b . The array `neutron(i, j, k)` is then assigned the following values:

$$\text{neutron}(i, j, k) = \begin{cases} \text{TRUE}, & \text{if } \text{ran} < f_b \\ \text{FALSE}, & \text{if } \text{ran} > f_b \end{cases} . \quad (3.17)$$

In the next step we have to decide about the existing bonds in the lattice. The bond status is implemented in the form of a four-dimensional logical array,

$$\text{connected}(\text{maxn}, \text{maxn}, \text{maxn}, 3),$$

which gives the existing bonds at every vertex in the three spatial directions. For populating the edges with bonds, we essentially proceed in the same way as in the case of the sites, by sweeping through the lattice and calling the random number generator at each edge. However there is one difference. Using `neutron(i, j, k)`, we first have to decide whether we have an edge with different endvertices or one that connects two sites of the same flavor. The program then assigns

$$\text{connected}(i, j, k, x) = \begin{cases} \text{TRUE}, & \text{if } \text{ran} < p \\ \text{FALSE}, & \text{if } \text{ran} > p \end{cases} , \quad (3.18)$$

where, in the case of $x = 3$, which is the positive z-direction,

$$p = \begin{cases} p_{=}, & \text{if } \text{neutron}(i, j, k) = \text{neutron}(i, j, k+1) \\ p_{\neq}, & \text{if } \text{neutron}(i, j, k) \neq \text{neutron}(i, j, k+1) \end{cases} . \quad (3.19)$$

We use free boundary conditions, so that all values of `connected(i, j, k, x)` on the boundaries are initialized as **FALSE**:

$$\begin{aligned} \text{connected}(n, i, j, 1) &= \text{FALSE} \\ \text{connected}(i, n, j, 2) &= \text{FALSE} \\ \text{connected}(i, j, n, 3) &= \text{FALSE}, \quad i, j \in [1, n] \end{aligned} \quad (3.20)$$

Furthermore a third array, an integer value array this time, is used to save the information on the cluster status of every vertex. The integer value assigned to every

entry of `clusterNumber(0:maxn1,0:maxn1,0:maxn1)` is the number corresponding to the place in row at which the cluster find algorithm, see Sec. 3.3.2, found the cluster to which the present vertex belongs. Here $\text{maxn1} = \text{maxn} + 1$. The value `clusterNumber(i,j,k) = 0` is meant to indicate that (i, j, k) has not yet been checked by the algorithm. The zeroth and $n + 1$ st layer vertices (in each direction) are assigned cluster numbers $hcln$ equal to the highest number of clusters occurring if the lattice is fully fragmented, plus one:

$$hcln = n^3 + 1. \quad (3.21)$$

This provides for a ‘surface cluster’ that seems already checked, which lets the cluster algorithm stop at the natural lattice boundaries. In the next step the lattice configuration is analyzed with the cluster find algorithm and the appropriate values are recorded. The whole Monte Carlo step is repeated n_{event} times, using independent random number seeds each time, which are obtained from the system clock, with n_{event} on the order of 100. Then the averages of the observables are calculated.

3.3.2 Cluster Analysis

We use a cluster algorithm first described in [BPDM86]. We abide by the same notation as used in the cited reference for the description of the algorithm. The set of all vertices in the lattice is denoted by A . The set of vertices that have not yet been checked by the cluster find algorithm and are thus still uncounted, is written as $A^{(0),i}$, with $A^{(0),i} \subset A$. The task is to find all clusters C_k and record their size $|C_i|$. The algorithm accomplishes this task by scanning the lattice for the first vertex \vec{z}_1^i belonging to the subset of unchecked vertices: $\vec{z}_1^i \in A^{(0),i}$. Now all other sites $\vec{z}_j^i \in A^{(1),i}$, connected by open edges to \vec{z}_1^i , $\vec{z}_j^i \longleftrightarrow \vec{z}_1^i$ have to be detected. $A^{(1),i}$

denotes the next generation of unchecked sites,

$$A^{(1),i} = A^{(0),i} - C^{(0),i}.$$

$C^{(0),i} = \{\bar{z}_1^i\}$ is called the zeroth generation of C_i , where $C_i = \{\bar{z}_1^i \dots \bar{z}_n^i\}$ is the cluster with $|C_i| = n$ which we want to detect. In the next step all previously unvisited neighbors of \bar{z}_1^i are checked if they are connected to the site from which the search is originating. All neighboring sites that are connected to \bar{z}_1^i form the so-called first generation $C^{(1),i}$ of C_i . At some n we will have

$$A^{(n+1),i} = A^{(n),i} - C^{(n-1),i} = A^{(n),i},$$

as $C^{(n),i} = \emptyset$, which is the termination condition for the algorithm. The cluster C_i is then given by

$$C_i = \bigcup_n^{l=0} C^{(l),i}. \quad (3.22)$$

The algorithm restarts screening the lattice until a new starting vertex \bar{z}_1^{i+1} , belonging to $A^{(0),i+1} = A^{(0),i} - C_i$, is found. All clusters have been found if $A^{(0),N} = \emptyset$ and N is then the number of clusters in the present configuration.

3.3.3 Determination of the Critical Value

The second type of program written is aimed at the question of determining the critical value in a more precise manner than from extrapolation methods based on phase transition plots, of, for example, p_∞ . Three different versions of this type of program have been written, which determine the threshold for the onset of percolation in terms of p_+ , p_- and f_b . In the description here, we will only describe the one that gives p_+^c through determining p_-^c . The first steps in all three programs are the same as described in Sec. 3.3.1, in that sense as that the procedure to populate the lattice

and the edges are the same. They stand, however in a different framework, which is described in the following. Every Monte-Carlo step now comprises an nested interval method approach to the critical value. We repeat each Monte Carlo step n_{event} times, with n_{event} again on the order of 100 and using different random seeds for each Monte Carlo step. For each value of f_b the program is given the values of p_{\neq} that are to be probed as well as a start interval for $p_{=} \in [a, b]$. The actual value of $p_{=}$ that is to be probed in the first sweep of the lattice is determined according to

$$p_{=} = c = \lambda b + (1 - \lambda) a. \quad (3.23)$$

A typical value that we used for λ was

$$\lambda = 0.9.$$

With the random number assigned for this Monte Carlo step the lattice is populated and the edges determined to be open or closed. Then, the cluster find algorithm, as described in Sec. 3.3.2, goes through the lattice. This time, however, as the aim is to determine the critical value, not the whole cluster information is needed, the only interesting question is whether there exists an infinite cluster as defined in Sec. 2.4.1 with (2.10) and (2.11). Therefore, the cluster find algorithm is constrained to one boundary layer of the lattice in one direction, which in the program is the (i, j, n) , $i, j \in [1, n]$ layer. From there, the algorithm follows the branching of every cluster but stops immediately if it reaches the bottom of the lattice, that is the $(i, j, 1)$, $i, j \in [1, n]$ layer. We then only have two possibilities: Either the algorithm stops after checking all clusters originating in the (i, j, n) , $i, j \in [1, n]$ layer and not finding any spanning cluster, where we assign $\psi = 0$ or it stops after finding a spanning cluster and $\psi = 1$ is assigned. Then the new $p_{=}$ -interval is

$$\begin{cases} [a, c], & \text{if } \psi = 0 \\ [c, b], & \text{if } \psi = 1 \end{cases} \quad (3.24)$$

This process is repeated a desired number of times, depending on the size of the final interval one wants to attain. Usually, we set as final interval size

$$|d - c| = 10^{-4},$$

where

$$d = \begin{cases} a, \\ b, \end{cases}$$

depending on the outcome of the last step. The value of c_{final} from the final step then gives the critical value

$$p_{=}^{c,i} = c_{final}. \quad (3.25)$$

After completion of the n_{event} Monte-Carlo steps averaging over all obtained $p_{=}^{c,i}$ yields the threshold:

$$p_{=}^c = \frac{1}{n} \sum_{i=1}^n p_{=}^{c,i}. \quad (3.26)$$

The critical value of the scaled control parameter p_+ is then simply given as

$$p_+^c = \alpha_{=} p_{=}^c + \alpha_{\neq} p_{\neq}^c. \quad (3.27)$$

A calculation of the statistical errors is performed as well. However, to obtain the total error, the systematic error, due to finite size effects, has to be added to the statistical errors. We will come back to a discussion of the systematic errors and ways to estimate them in Sec. 3.7.

3.4 Two Components using the Scaled Control Parameter

After giving a review of the techniques used in the simulations of which we present the results, we now want to come back to the discussion led in Sec. 3.1. In (3.6) we

introduced a scaled control parameter with the intention of being more capable to extract information about a possible phase transition and to be able to describe the phase transition behavior in terms of just one variable. In Sec. 3.2 we then discussed our model, in the case of two components, still in terms of two variables p_- and p_+ . Now we want to realize a description in terms of the variable p_+ .

3.4.1 Entire Parameter Range

First, we will aim at a discussion of the data from simulations where, as before, $f_b = 0.5$ and then come to present the results for $f_b \neq 0.5$.

Blue Species Concentration $f_b = 0.5$

We take the same data as shown in Fig. 3.1, that is, we have $p_-, p_+ \in [0, 1]$ and analyze it in terms of the scaled control parameter p_+ . The result is shown in Fig. 3.4. Two

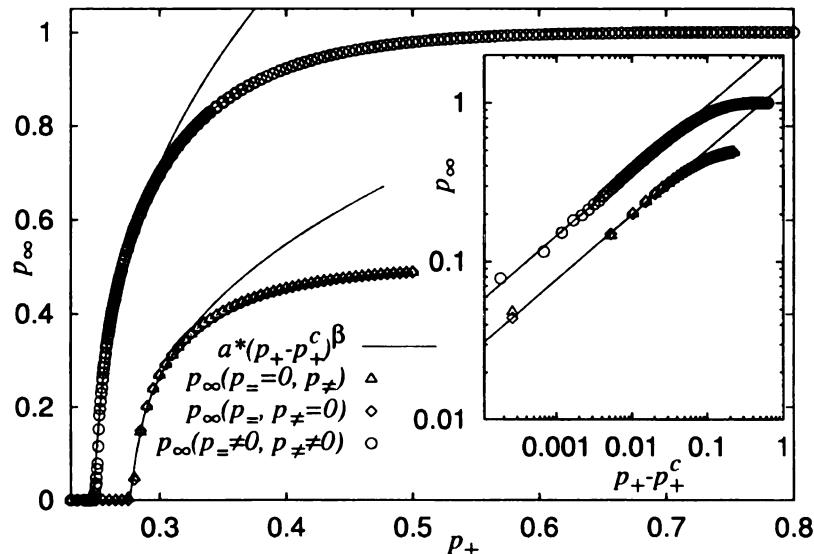


Figure 3.4: Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter, p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, for values of $p_-, p_+ \in [0, 1]$, fitted with $p_\infty \propto (p_+ - p_+^c)^\beta$ (solid line). Here $p_+^c \simeq 0.251$ for the 'upper' branch, $p_+^c \simeq 0.280$ for the 'lower' branch and $\beta = 0.41$ in both cases. The inset shows the same data in a double logarithmic representation.

distinct branches can be seen, both in the shape of a second order phase transition. Fig. 3.4 first suggests that the scaled control parameter p_+ is a good variable, as we only have two universal scaled curves. However, it suggests too, that some other phase transition happens in the system as well. On a first eye-analysis it seems that we see the system in two different states, which both show, as a function of p_+ , a similar behavior in the percolation probability p_∞ . Before we come to an analysis about how the two phases, of which the two universal scaled curves are an indicator, come about, we will devote some time to an analysis of the curves themselves.

In the main part of Fig. 3.4 we show the data on linearly scaled axes. Both are in the form of a second order phase transition and we fit both curves with the expectation from ordinary one component percolation theory, see (2.67),

$$p_\infty = a (p_+ - p_+^c)^\beta. \quad (3.28)$$

With the fitting procedure, we find for the critical value of the 'upper branch'

$$p_+^c = 0.251 \pm 0.002. \quad (3.29)$$

Taking finite size effects into account, for which we did not correct at this point, this stands in reasonable agreement with other numerical results for one component bond percolation theory, see for example, [SA94], which state

$$p_+^c = 0.2488, \quad (3.30)$$

or [LZ98], where the threshold is given very precisely as

$$p_+^c = 0.2488126 \pm 0.0000005. \quad (3.31)$$

The value of the lower branch, however, is shifted to a higher threshold. With the same fitting procedure we find for the critical value of the data belonging to the 'lower

branch'

$$p_+^c = 0.280 \pm 0.002. \quad (3.32)$$

Another important quantity that should elucidate the situation is the critical exponent β . To test upon it, we print the same data as shown in the main part of Fig. 3.4 in a double logarithmic plot, the result of which is shown in the inset of Fig. 3.4. We can see that in the double logarithmic display both branches are well-fitted by linear functions with the same slope β , that is, on a linear scale with the same critical exponent, which we find to be

$$\beta = 0.41, \quad (3.33)$$

for both branches. This is the same critical exponent as found by other authors for one-component bond percolation theory and as given, for example, in [SA94]. We should note again that the critical value of p_+ depends on the dimension and the lattice structure of the system, whereas the critical exponents just depend on the dimensionality.

We now come back to the question which two states we see manifest in form of the two p_∞ curves. A further analysis of the data unveils that the 'upper branch' constitutes of points with both p_+ and p_- non-zero¹, whereas all points with ($p_+ = 0, p_- \neq 0$) and ($p_+ \neq 0, p_- = 0$) fall on the 'lower' branch. In a shorter notation we can summarize this behavior in the following way

$$p_+ p_- \neq 0, \quad \text{'upper branch'} \quad (3.34)$$

$$p_+ p_- = 0, \quad \text{'lower branch'} \quad (3.35)$$

This leads to the conclusion that some fundamental change has to take place in the

¹We have to note that the term 'non-zero' is somewhat imprecise, we will further elaborate this point in Sec. 3.5.2

system, when the system is brought to either one of the two limits

$$p_{=} \rightarrow 0,$$

or

$$p_{\neq} \rightarrow 0.$$

Together with the results stated above we can now conclude that, as long as both bond types are active, which corresponds to the $(p_{=} \neq 0, p_{\neq} \neq 0)$ -regime, the two-component site-bond percolation system under observation here and the ordinary one-component bond percolation system show an identical phase transition behavior, which is in accordance with the findings presented in [Baued]. Obviously this means further that the actual values of the individual bond existence probabilities $p_{=}$ and p_{\neq} do not have a direct influence on the percolation probability, but rather that the actual bond density p_{+} is the direct equivalent of the control parameter in one-component percolation and thus fulfills the expectations under which it was introduced. As soon as one of the bond types is disabled, however, the system fundamentally changes its behavior, going over to a new critical value of p_{+} for the order parameter p_{∞} . The basic features are retained, a second order phase transition of the order parameter, p_{∞} , is still observed and furthermore with the same critical exponent β as in the non-zero regime of $p_{=}$ and p_{\neq} .

Blue Species Concentration $f_b \neq 0.5$

Probing at another value of f_b yields essentially the same effect. As an example, in Fig. 3.5, we show data for $f_b = 0.3$. Here, the curve that we called 'upper branch', that is the data for values $p_{=} \neq 0$ and $p_{\neq} \neq 0$ can be shown to be exactly the same as in the previous case, where $f_b = 0.5$, we retain precisely the same critical value

$$p_{+}^c \simeq 0.251$$

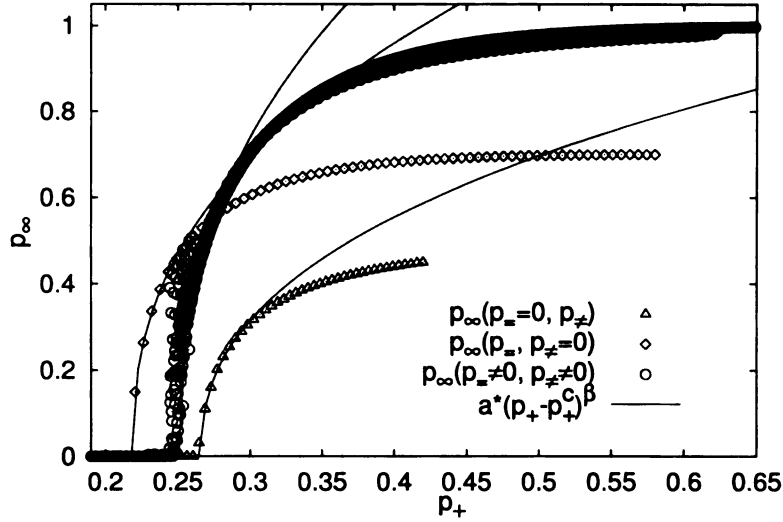


Figure 3.5: Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter, p_+ , in a 128^3 simple cubic lattice with $f_b = 0.3$, for values of $p_-, p_\neq \in [0, 1]$, fitted with $p_\infty \propto (p_+ - p_+^c)^\beta$ (solid line). Here $p_+^c \simeq 0.251$ for the 'upper' branch, $p_+^c \simeq 0.218$ for the $p_\neq = 0$ branch, $p_+^c \simeq 0.266$ for the $p_- = 0$ branch and $\beta = 0.41$ in all cases.

and the same critical exponent β . For the data that constitutes of points where either $p_- = 0$ or $p_\neq = 0$, the situation is changed. First, the data for $p_- = 0$ and $p_\neq = 0$ do not fall on the same universal scaled curve, but rather show different limiting values for $p_+ \rightarrow 1$ and different critical values². We find

$$p_+^c(p_- = 0, p_\neq) = 0.266 \pm 0.002. \quad (3.36)$$

for the ' $p_- = 0$ '-branch and

$$p_+^c(p_-, p_\neq = 0) = 0.218 \pm 0.002. \quad (3.37)$$

for the ' $p_\neq = 0$ '-branch. In Fig. 3.6 we show the same data³ as depicted in Fig. 3.5 in a double-logarithmic plot. As can be seen, all three curves are very well fit with

²When we say $p_+ \rightarrow 1$ limit here, we mean to indicate the direction in which we let p_+ go, being well aware that $p_+ = 1$ can not be attained for most values of f_b whilst $p_- = 0$ or $p_\neq = 0$.

³We have to note that, since the data shown in Fig 3.5 is lower quality data then the one depicted in Fig. 3.4, we have, in Fig. 3.6, corrected for some of the stronger fluctuations seen in Fig. 3.6 and left out some data points

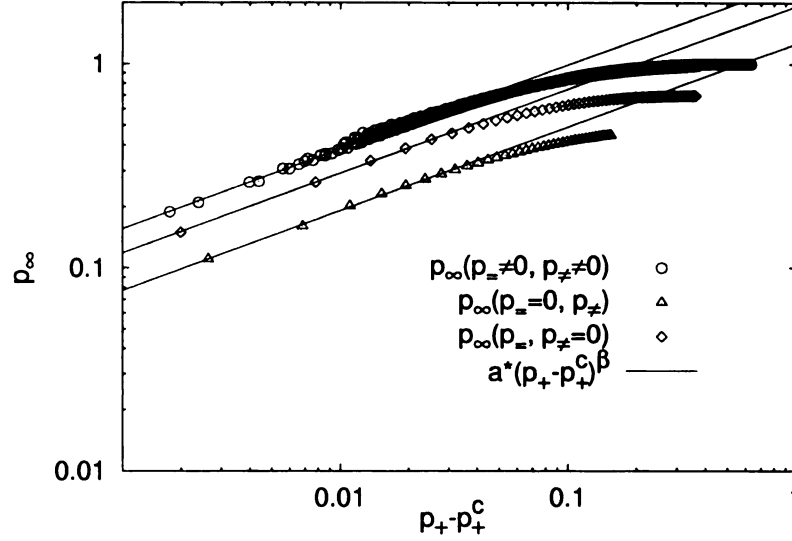


Figure 3.6: The same data as shown in Fig. 3.5 in a double logarithmic representation, with a slope of all three curves of $\beta = 0.41$.

linear functions of the same slope β , that is the same critical exponent β in the linear scale. As was already the case for $f_b = 0.5$, we again have

$$\beta = 0.41, \quad (3.38)$$

for all three branches. A different behavior in the limiting values of p_+ and the critical value p_+^c for the ' $p_+ = 0$ '-branch and the ' $p_+ \neq 0$ '-branch has to be expected, since in the system, we have a symmetry in the concentration with respect to $f_b = 0.5$. This symmetry is made possible through us setting

$$p_+ = p_{bb} = p_{rr},$$

which leaves edges connecting two sites of the same species and edges connecting two sites of different species as only possibilities. We then have a 'binary' system with α_+ and α_- as the two quantities that show a symmetry with respect to $f_b = 0.5$ and furthermore have

$$\alpha_+(f_b = 0.5) = \alpha_-(f_b = 0.5),$$

see (3.14), (3.15) and Fig. 3.7, which leads to the coinciding of the ($p_{=} = 0, p_{\neq} \neq 0$) and ($p_{=} \neq 0, p_{\neq} = 0$) curves as shown in Fig. 3.4. The fact that the limiting values

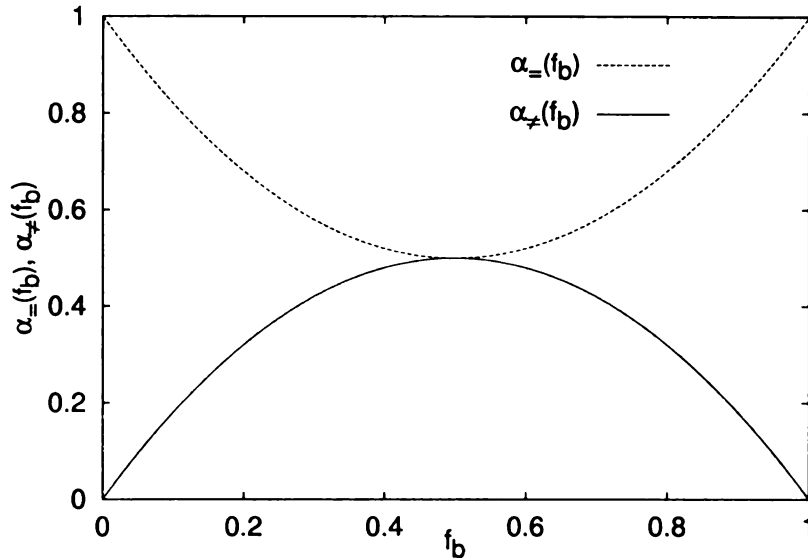


Figure 3.7: The normalized density of edges connecting two sites of equal flavor, $\alpha_{=}(f_b)$ and the normalized density of edges connecting two sites of different flavor, $\alpha_{\neq}(f_b)$. See also (3.14) and (3.15).

$p_{\infty}(p_{+} \rightarrow 1)$ of both curves differ can be understood in the following way. Having set $p_{=} = 0$ and letting $p_{+} \rightarrow 1$ requires letting $p_{\neq} \rightarrow 1$. Then the maximum value of p_{∞} is determined by f_b :

$$p_{\infty}(p_{=} = 0, p_{\neq} = 1) = \min(f_b, (1 - f_b)), \quad (3.39)$$

with a symmetry again with respect to $f_b = 0.5$. The same line of thought applies to the case where $p_{\neq} = 0$ and $p_{=} = 1$, however due to the behavior of $\alpha_{=}$ we have

$$p_{\infty}(p_{=} = 1, p_{\neq} = 0) = \max(f_b, (1 - f_b)). \quad (3.40)$$

It has to be noted that the equality in (3.39) and (3.40) is not strict, since geometrical effects play an important role. By geometrical effects we mean the fact that due to the geometric position of the particles on the lattice some of the particles will be inaccessible by either, depending on the limit, bb -, rr - or br -bonds and thus a part

of the whole fraction f_b or $f_r = (1 - f_b)$ will be excluded. We want to elaborate on the footnote (2) made above to clarify the notation $p_+ \rightarrow 1$. Having set one of the bond existence probabilities equal to 0, the maximum value of p_+ is given by α_+ or α_- respectively. Thus, unless $f_b = 0$ or $f_b = 1$ the real limit $p_+ = 1$ can never be reached once either $p_+ = 0$ or $p_- = 0$, rather will it be impossible to probe above a maximum value of p_+ , which is given as

$$p_+^{max} = \alpha_+,$$

or

$$p_+^{max} = \alpha_-,$$

depending on whether $(p_+ = 0, p_- = 1)$ or $(p_+ = 0, p_- = 1)$ was set.

3.5 The Percolation Probability

In the afore-held discussion on the behavior of the percolation probability as a function of the scaled control parameter p_+ it became clear that in a wide range of values of the 'contributing' parameters p_+ and p_- the percolation probability exhibits features similar to the ones observed for the percolation probability in an ordinary one-component bond percolation system, but that when setting one of the contributing parameters to zero, the system would behave different. In this section we want to present results that show how this different behavior comes about. We will more or less focus on the limit $p_- = 0$, as the same line of arguments applies in the $p_+ = 0$ limit, but we will still present the results from an investigation in the second limit too.

3.5.1 $p_- \rightarrow 0$ Limit

Going back to Fig. 3.4 we can choose an arbitrary value of $p_+ > p_+^c$ ('lower branch'), so that the corresponding percolation probabilities will be non-zero and compare the

percolation probability that we have on the upper branch with the one that one obtains through the lower branch. One realizes that there exists a finite difference:

$$p_\infty(p_= \neq 0, p_\neq \neq 0) - p_\infty(p_=, p_\neq = 0) > 0. \quad (3.41)$$

The question arises, how the percolation probability behaves when the system is let into the $p_\neq = 0$ limit.

For simplicity, we first choose

$$p_= = 1.$$

We will furthermore, for the sake of ease of argument, set

$$f_b = 0.5$$

in this first discussion and then later on state the differences that occur for other values of f_b . Then setting $p_\neq = 0$ corresponds to a lattice in which all available bb -edges and all available rr -edges are open, but all br -edges are closed. With a very high probability there will be an infinite network present. This comes about in the following way. Effectively with this choice of parameters, we are modeling a two-component site percolation model with two disjunct types of clusters. These are clusters of b -type and clusters of r -type, which are entirely disconnected as $p_\neq = 0$ was chosen. Then, for site percolation, for the given f_b , we are above the site percolation threshold in the case of a simple cubic lattice, which is, compare [SA94],

$$f_{site}^c = 0.3116. \quad (3.42)$$

Since the second species has a concentration $f_r = (1 - f_b) > f_{site}^c$ above the threshold as well, it is highly probable that both species will have a spanning cluster. According to the definition we set forth for an infinite cluster (2.10) and (2.11), there will be only one infinite cluster C_∞ , however, which has to fulfill the additional requirement

of being the biggest cluster. Let us just assume that the biggest, spanning cluster, which we identify with the infinite cluster, is of blue color. Following (2.66) and (2.65), we can express the percolation probability as

$$p_\infty(p_\neq = 0) = f_b - \sum_{s=1}^{\infty-1} n_s^b s, \quad (3.43)$$

where, like before, the symbolic notation ' $\infty - 1$ ' for a finite system is meant to indicate that in the sum the infinite cluster is excluded. From a simple argument, we can approximately evaluate the sum, without exactly calculating every term in the cluster size distribution n_s^b . Given the fact that $p_ = 1$ and $p_\neq = 0$, according to the argument presented in the preceding section, see (3.40), we will encounter a maximum value of p_∞ ,

$$p_\infty^{max} = f_b = 0.5. \quad (3.44)$$

It has to be noted that this value is an upper limit, typically the percolation probability will come to lie slightly below this value, as confirmed in simulations, where we find

$$p_\infty \approx 0.48. \quad (3.45)$$

The reason are geometrical effects. By geometrical effects it is meant that some blue sites will be inaccessible from other blue sites, thus leading to the fact that not the whole fraction of f_b blue sites is accessible. In (3.43) n_s^b denotes the number of b -clusters of size s . As already stated, there is a high probability that also the second color has a spanning cluster. If not so, then at least the biggest r -cluster, C_{max}^r , will have a size on the order of the size of the infinite cluster, since both colors are symmetric,

$$|C_{max}^r| \approx |C_\infty|. \quad (3.46)$$

Analogously to (3.43) we can formulate the probability that a given lattice site is part of the biggest r -cluster, C_{max}^r , as

$$p_{max}^r(p_{\neq} = 0) = f_r - \sum_{s=1}^{max-1} n_s^r s, \quad (3.47)$$

and with the same line of thought as for the blue species we find

$$p_{max}^{r,max} = f_r = 0.5. \quad (3.48)$$

Again, the true value will be slightly below that, where, again,

$$p_{max}^r \approx 0.48, \quad (3.49)$$

is a typical value. Starting from this configuration where $p_{\infty} \lesssim 0.5$, and $p_{max}^r \lesssim 0.5$, we now set

$$p_{\neq} = \varepsilon \quad (3.50)$$

$$> 0.$$

This will introduce a very low br -bond density in the lattice. The infinite cluster in this new configuration of parameter values can then consist of both b - and r -vertices and we can write the percolation probability p_{∞} as

$$p_{\infty}(p_{\neq} = \varepsilon) = 1 - \sum_{s=1}^{\infty-1} n_s s. \quad (3.51)$$

This yields a difference in the percolation probability at $p_{\neq} = 0$ and the percolation probability at $p_{\neq} = \varepsilon$:

$$\begin{aligned} \delta_{\infty}(\varepsilon) &= p_{\infty}(p_{\neq} = \varepsilon) - p_{\infty}(p_{\neq} = 0) \\ &= 1 - \sum_{s=1}^{\infty-1} n_s s - \left(f_b - \sum_{s=1}^{\infty-1} n_s^b s \right). \end{aligned} \quad (3.52)$$

By rewriting the concentration of the blue species, f_b , as

$$\begin{aligned} f_b &= (1 - f_r) \\ &= 1 - \sum_{s=1}^{max} n_s^r s, \end{aligned} \quad (3.53)$$

we obtain

$$\delta_\infty(\varepsilon) = \left(\sum_{s=1}^{\infty-1} n_s^b s + \sum_{s=1}^{max} n_s^r s \right) - \sum_{s=1}^{\infty-1} n_s s. \quad (3.54)$$

The difference δ_∞ has the property that, if we let $\varepsilon \rightarrow 0$, for all $\varepsilon > 0$, the limit will be non-vanishing:

$$\lim_{\varepsilon \rightarrow 0} \delta_\infty(\varepsilon > 0) > 0. \quad (3.55)$$

This comes about, since, with a very high probability, the bonds making up for this low density will connect the two biggest clusters in the lattice, C_∞ and C_{max}^r , as according to our consideration above, we have,

$$p_\infty + p_{max}^r \lesssim 1. \quad (3.56)$$

Thus almost surely do we have (3.55) fulfilled.

How is the situation in a simulation on a finite lattice? In this case the situation is slightly different. Setting the bond probability p_\neq to some fixed value $p_\neq > 0$ does yield a corresponding bond density, but just on average. Events where no bonds at all are introduced in the lattice do have finite probabilities. What is the implication? Let us consider a case where we set

$$\begin{aligned} p_\neq &= \varepsilon \\ &= \frac{1}{N_{edges}}, \end{aligned} \quad (3.57)$$

which introduces *on average* one bond $\langle \vec{b}, \vec{r} \rangle$ in the lattice. For each event where such a *br*-bond does occur, almost surely $\langle \vec{b}, \vec{r} \rangle$ will connect the infinite cluster C_∞ and the biggest cluster of the red colored species, C_{max}^r . We rely on the same argument as above, which states that we have probabilities to belong to the infinite cluster and to belong to the biggest red cluster, both close to 0.5,

$$p_\infty + p_{max}^r \lesssim 1.$$

Then, the 'new' infinite cluster will be made up out of the 'former' C_∞ and C_{max}^r together. This will yield, as in the case of the infinite lattice, a higher percolation probability compared to the $p_\neq = 0$ system. The rare events in which the br -bond $\langle \vec{b}, \vec{r} \rangle$ does not connect C_∞ and C_{max}^r or where it connects C_∞ to some finite r -cluster, C_{fn}^r , as well as the events in which no br -bond at all is formed, will exhibit a smaller increase in the percolation probability or none at all. In a simulation an average over all events will yield an effective value of δ_∞ , denoted by δ_∞^{eff} , with

$$0 < \delta_\infty^{eff} < \delta_\infty. \quad (3.58)$$

The arguments presented, with (3.55) for the infinite lattice and (3.58) for the finite lattice, lead to the conclusion that in the limit $p_\neq \rightarrow 0$ a first order phase transition takes place in p_∞ .

The simulation results support this conjecture, as shown in Fig. 3.8. It has to be

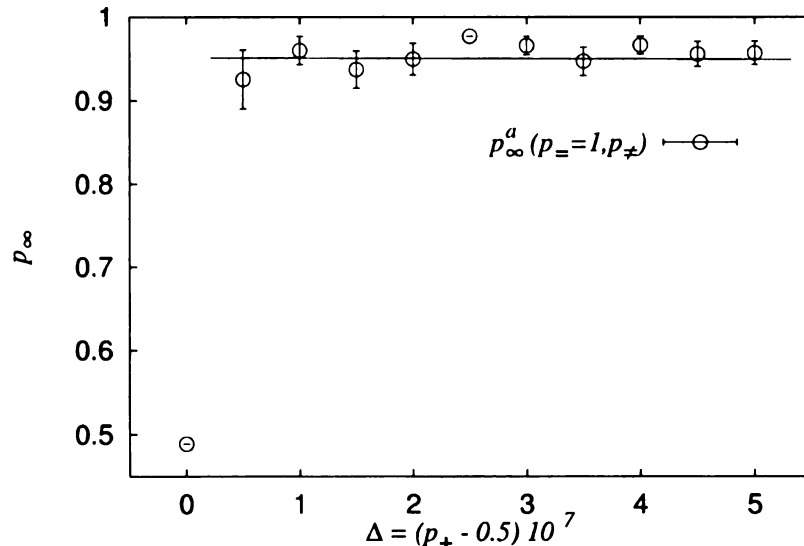


Figure 3.8: Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_+ = 1$ for varied p_\neq . 50 independent simulation events were taken into account and the average was taken over events in which the number of br -bonds actually formed in the simulation, n_{br} , was non-zero.

noted that for the data shown here in the analysis the average was taken only over

events in which the number of br -bonds, n_{br} , actually produced in the simulation, was non-finite:

$$n_{br} \neq 0.$$

Another possibility is to average over all events, which gives a smaller δ_{∞}^{eff} , as one also includes events in which the lattice is completely unchanged and the same percolation probability is found. Data from the same simulation, analyzed with the second averaging technique, where all events were taken into account, is shown in Fig. 3.9. Naturally the question arises, what the behavior is like for $p_{\pm} \neq 1$. Still, a first order

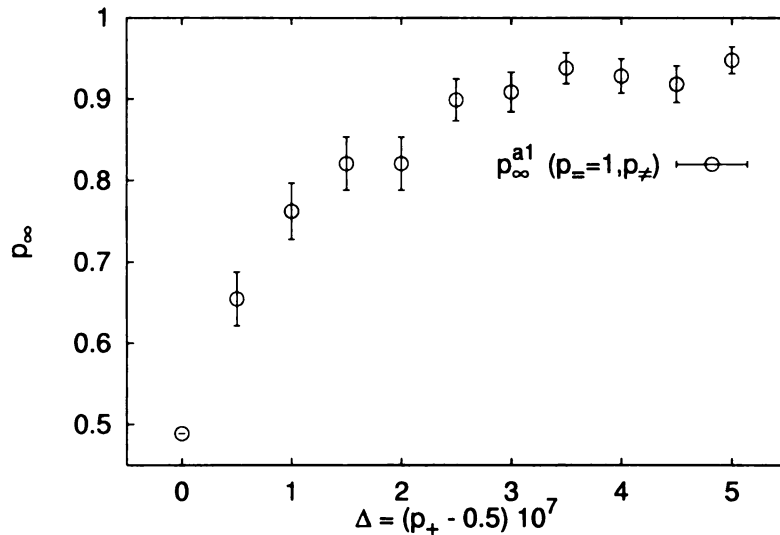


Figure 3.9: Probability to belong to the infinite cluster, p_{∞} , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_{\pm} = 1$ for varied p_{\neq} . 50 independent simulation events were taken into account and the average was taken over all events.

phase transition will be observed, since essentially nothing is changed, compared to the case where $p_{\pm} = 1$. The effect will be somewhat less pronounced, that is a smaller δ_{∞} will be seen. This comes about since

$$|C_{\infty}(p_{\pm} < 1)| < |C_{\infty}(p_{\pm} = 1)|,$$

and

$$|C_{max}^r(p_{=} < 1)| < |C_{max}^r(p_{=} = 1)|.$$

It is clear, however that

$$p_{=} > \frac{p_+^c(p_{=} \neq 0, p_{\neq} \neq 0)}{\alpha_{=}(f_b)} \quad (3.59)$$

is necessary to obtain this phase transition, as otherwise

$$p_{\infty} = 0.$$

Equation (3.59) represents a condition $p_{=}$ and f_b combined are subjected to. For

$$\frac{p_+^c(p_{=} \neq 0, p_{\neq} \neq 0)}{\alpha_{=}(f_b)} < p_{=} < \frac{p_+^c(p_{=}, p_{\neq} = 0)}{\alpha_{=}(f_b)} \quad (3.60)$$

the above argument, which relies on the existence of an infinite cluster in the $p_{\neq} = 0$ limit does not hold anymore in exactly the same way. However we merely have to replace the term 'infinite cluster C_{∞} ' by 'biggest b -cluster' and then rely on the same conduct of argument again. There will be no percolation being realized with $p_{\neq} = 0$, but connecting C_{max}^b (instead of C_{∞} , as before) with C_{max}^r at $p_{\neq} = \varepsilon$ creates an infinite br -cluster. In the case of $p_{=}$ satisfying (3.60), the effect will be diminished, as already explained afore, as the sums in (3.54) turn out smaller.

What is the situation like for $f_b \neq 0.5$? In order to have the original argument hold for $p_{=} = 1$, the system has to stay above the site percolation threshold as given in (3.42). Below, the same consideration as above applies, there will only be finite clusters present and again, the term infinite cluster has to be replaced by biggest finite cluster to follow the same line of argument. The first order phase transition exhibits a smaller discontinuity with decreasing f_b for

$$f_b < 0.5,$$

or with increasing f_b for

$$f_b > 0.5,$$

and the effect continuously vanishes for $f_b \rightarrow 0$ and $f_b \rightarrow 1$.

3.5.2 The 'Smearing-Out' Effect

Some arguments of the discussion from the preceding section can be applied in the question of an effect that we call 'smearing-out' effect, which we already briefly commented on in a footnote in Sec. 3.4.1. The observable we are interested in is the percolation probability p_∞ . We set p_\neq and $p_=\text{ to some fixed value } p_=\text{, } p_\neq \in [0, 1]$, and determine the percolation probability. We then show the percolation probability p_∞ as a function of p_\neq and take $p_=\text{ as parameter, the result of which is shown Fig. 3.10}^4$. It is noteworthy that we transformed the real parameter dependence on $p_=\text{ that was present in the simulation to a parametric dependence on } p_+\text{ since then the known values of thresholds are more easily compared. What leads to the functional forms depicted in Fig. 3.10? At } p_+ = 0.25\text{ there exist only finite } b\text{- and } r\text{-clusters, since the system is below the threshold, } p_+^c \approx 0.28\text{. Then, increasing } p_\neq\text{ only connects finite clusters, leading to a small } \delta_\infty\text{, leading to the nearly continuous looking function. For a slightly higher value of } p_+ = 0.26\text{ the effect is quite more important and yet more astounding is the change from the curve where } p_+ = 0.26\text{ to the one for } p_+ = 0.28\text{, where the claim of a first order phase transition seems more obvious than in the cases cited before. For completeness we also show curves for } p_+ = 0.30\text{ and } p_+ = 0.5\text{, where it becomes clear that the } \delta_\infty\text{ observed keeps becoming bigger with increased } p_+\text{. At the same time, the width of the transition region, where effects discussed above in the context of } \delta_\infty^{eff}\text{ are of importance, becomes increasingly smaller. This transition$

⁴We would like to note that the small 'hole' in the 'right hand side' of the simulation data is no inherent effect, but rather due to a lack of simulation in this region, which however is symmetric to the 'left hand side' of the curves.

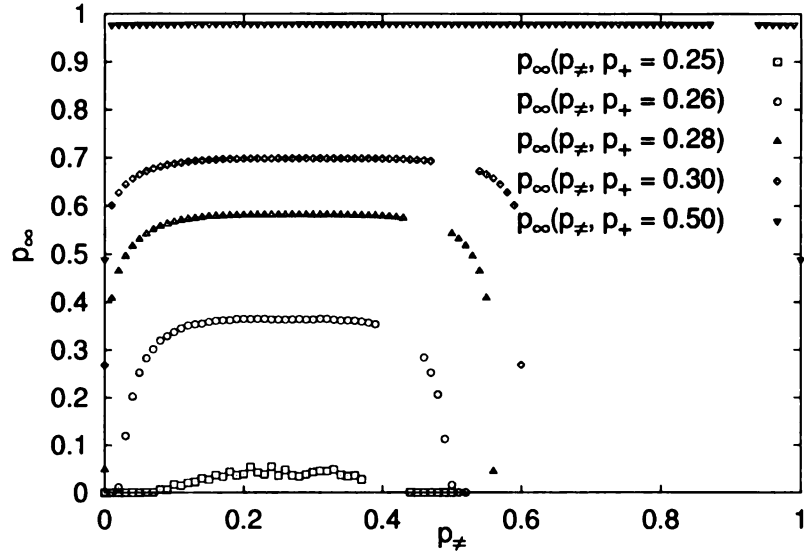


Figure 3.10: Percolation probability as a function of p_{\neq} , with a parametric dependence on p_{+} , shown for a 128^3 simple cubic lattice with $f_b = 0.5$.

region and its width have an effect when the percolation probability is shown as a function of p_{+} . It causes the two 'branches' shown in Fig. 3.4 not to be clear, but 'smeared out' around the most probable 'plateau' value observed in Fig. 3.10. In Fig. 3.4 we corrected for this smearing out by only taking into account data points lying on the 'plateau' seen in Fig. 3.10. Thus we can now precise our notation of ' $p_{=}$ and p_{\neq} non-zero', clarifying that we mean values of $p_{=}$ and p_{\neq} chosen in such a way that the effect of the transition region, due to the first order phase transition having smaller discontinuities for smaller $p_{=}$ (smaller p_{+} in the figure), can not be seen, that is, values chosen in such a way that p_{∞} comes to lie in the plateau region.

3.5.3 $p_{=}$ \rightarrow 0 Limit

In this section we want to briefly show that the same results hold for $p_{=}$ \rightarrow 0 as in the preceding section for p_{\neq} \rightarrow 0. The backbone of the argumentation, which is the presence of two clusters of essentially the same size in the lattice at $p_{=}$ = 0, is retained, however the argumentation how they come about has to be changed.

Again, for ease of argument, we first set $p_{\neq} = 1$ fixed and vary $p_{=}$ from $p_{=} = 0$ to $p_{=} = \varepsilon$. For $(p_{=} = 0, p_{\neq} = 1)$ the situation will be as follows: There are only br -bonds allowed in the lattice, leading, with this combination of parameter values, to an infinite br -cluster C_{∞} . The percolation probability, p_{∞} , is given again, compare (3.39) and (3.44), by

$$p_{\infty} \lesssim f_b = 0.5. \quad (3.61)$$

Although, contrary to the $p_{\neq} = 0$ limit, no second species is left to provide a second cluster with a size on the order of the size of the infinite cluster C_{∞} , there is a second br -cluster present in the system that we denote by C_{max} and that, as was in the $p_{\neq} = 0$ limit the biggest red cluster to the biggest blue cluster (assumed to be the infinite cluster), is symmetric to the infinite cluster. Thus, with a very high probability, C_{max} spans the entire system as well. For C_{∞} and C_{max} we have

$$|C_{max}| \approx |C_{\infty}|, \quad (3.62)$$

yielding, as before,

$$p_{\infty} + p_{max} \lesssim 1. \quad (3.63)$$

How does C_{max} come about? This feature is unique to lattices where, from a given vertex z it is not possible to reach *every* other vertex z_j on the lattice with a path $z \longleftrightarrow z_j$ of length m odd *and* a path of length n even. This is the case for the simple cubic lattice. Starting from some blue vertex $z_i^b = (k, l, m)$, which coordinate integers satisfy

$$k + l + m = (2n + 1), \quad n \in \mathbb{N}, \quad (3.64)$$

it will be impossible to reach another blue vertex $z_j^b = (r, s, t)$ with

$$r + s + t = 2n, \quad n \in \mathbb{N}, \quad (3.65)$$

since in this configuration, with all bb - and rr -bonds disabled and only br -edges open, always an even number of bonds is needed to get from a vertex with one color to another vertex of the same color. Thus in this configuration clusters incorporating 'odd' vertices of one color and clusters incorporating 'even' vertices of the same color will be entirely disjoint, providing for the two systems that both have, with a very high probability, spanning clusters. If we now let

$$\begin{aligned} p_{=} &= \varepsilon \\ &> 0, \end{aligned} \tag{3.66}$$

a low density of bb - and rr -bonds is introduced in the lattice. The bond(s) introduced by $p_{=} = \varepsilon$ open, with a high probability, an edge connecting C_{max} and C_{∞} , leading to a non-vanishing δ_{∞} ,

$$\lim_{\varepsilon \rightarrow 0} \delta_{\infty}(\varepsilon > 0) > 0. \tag{3.67}$$

Another way of arguing, which is restricted to the special case where $f_b = 0.5$ involves the system as discussed in Sec. 3.5.1 and a symmetry transformation. Before we proceed to give the transformation, let us introduce some short notation. All operations are done in \mathbb{Z}/\mathbb{Z}_2 . The color of a vertex is denoted by

$$c(k, l, m) = \begin{cases} 0, & \text{if } (k, l, m) \text{ blue} \\ 1, & \text{if } (k, l, m) \text{ red} \end{cases}, \tag{3.68}$$

and we define the parity of a vertex as

$$p(k, l, m) = \begin{cases} 0, & \text{if } (k + l + m) = 2n, n \in \mathbb{N} \\ 1, & \text{if } (k + l + m) = (2n + 1), n \in \mathbb{N} \end{cases}. \tag{3.69}$$

The symmetry transformation is described by the following transformation rules:

$$p'_{=} = p_{\neq} \tag{3.70}$$

$$p'_{\neq} = p_{=} \tag{3.71}$$

$$c(k, l, m)' = c(k, l, m) + p(k, l, m). \tag{3.72}$$

This changes the color of every 'odd' blue and of every 'even' red vertex. This means that on average half of the blue species are changed to red and half of the red species are changed to blue. Thus the concentrations are preserved and obviously, by conserving the species concentrations $f_b = 0.5$ and $f_r = 0.5$, the densities of accessible edges, $\alpha_{=}(f_b)$ and $\alpha_{\neq}(f_b)$ are conserved too. Every br -edge gets transformed into a bb - or rr -edge and every bb - and rr -edge becomes a br -edge. Since, however, the bond probabilities $p_{=}$ and p_{\neq} are transformed according to (3.70), these edges get occupied with the same probability as the br -edges before. Thus, as already stated, (3.70) represents a symmetry transformation for the system where $f_b = 0.5$.

Applying this transformation to the special case ($p_{=} = 0, p_{\neq} = 1$) yields a transformation to the system discussed in Sec. (3.5.1), where ($p_{=} = 1, p_{\neq} = 0$) or vice-versa. Thus the simplest explanation of the behavior encountered here is to refer to the system discussed in Sec. 3.5.1 and to the arguments presented there and then transform the system with (3.70) to the system interested in in this section.

For simulations on finite lattices the slight changes in the line of argument as discussed in Sec. 3.5.1 apply, to which we merely want to refer at this point. We support the claim of conjecture (3.67) with Fig. 3.11, which reproduces the behavior shown in Fig. 3.8. The two methods of averaging discussed above are also applicable here, but, since Fig. 3.8 already exhibits the same features as Fig. 3.11 we restrict ourselves to this one averaging technique. In this limit here, ($p_{=} = 0, p_{\neq} = 1$), the system has to be above a different percolation threshold, f_b^c , see [HB99], which we will discuss in Sec. 3.6.5.

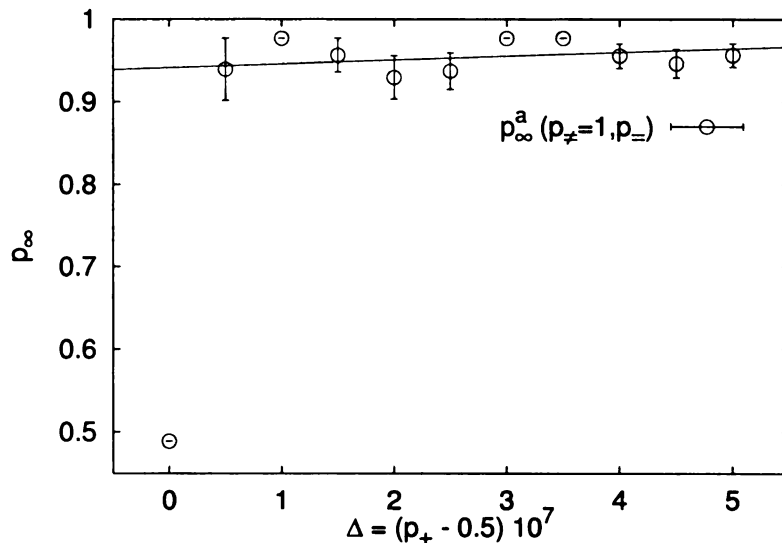


Figure 3.11: Probability to belong to the infinite cluster, p_∞ , as a function of the scaled control parameter p_+ , in a 128^3 simple cubic lattice with $f_b = 0.5$, at fixed $p_\neq = 1$ for varied $p_=$. 50 independent simulation events were taken into account and the average was taken over events in which the number of br -bonds actually formed in the simulation, n_{br} , was non-zero.

3.6 The Critical Value of the Scaled Control Parameter

Obviously the question arises, what the behavior of the critical value of the scaled control parameter, p_+^c , is like. In Sec. 3.4.1 the results presented pointed at a concentration dependence of the threshold. We will again, as already done in the previous section, first focus on the limit $p_\neq \rightarrow 0$ and then turn our attention to the case where $p_= \rightarrow 0$.

3.6.1 $p_\neq \rightarrow 0$ Limit

From Fig. 3.4 in Sec. 3.4.1 it was already clear that when setting the system into a limit in which only one type of edges can be open, the percolation threshold, or to be exact, the critical value of the scaled control parameter, p_+^c , would take a different value than in the case where all types of edges could be open. What Fig. 3.4

could not show was the way this transition came about. How is the critical value p_+^c transformed? In Sec. 3.5.1 we found that in the limit we focus on here, $p_{\neq} \rightarrow 0$, the percolation probability undergoes a first order phase transition. Is the same true for the percolation threshold? In a simulation specially aimed at answering this question, we set p_{\neq} to fixed values,

$$p_{\neq} \in [0, 1]$$

and then apply the algorithm described in Sec. 3.3.3, which uses the nested interval method, to determine the corresponding critical value of p_+ , p_+^c . With p_{\neq} and p_+^c the percolation threshold p_+^c can be calculated. We show the results in Fig. 3.12. It can be seen that the transition is continuous. Unlike the percolation probability,

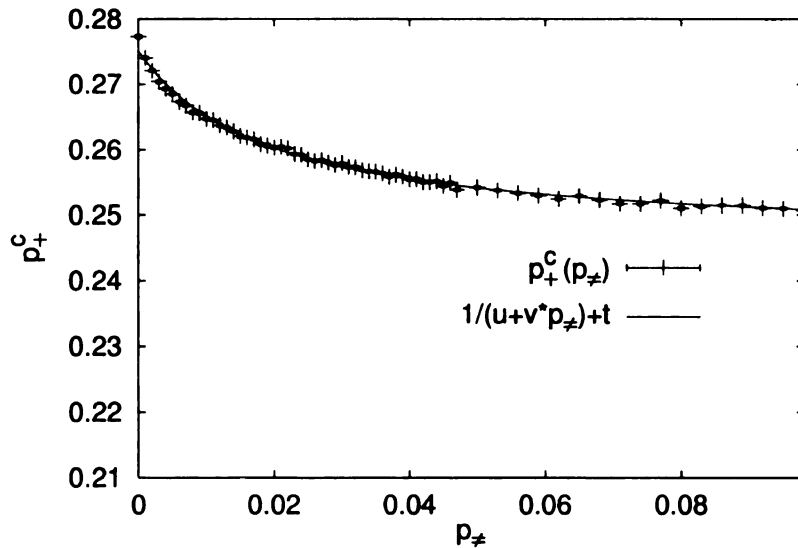


Figure 3.12: Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.5$, plotted as a function of p_{\neq} .

the percolation threshold p_+^c does not exhibit a discontinuity when $p_{\neq} \rightarrow 0$. In the Figure, we only show the interval $p_{\neq} \in [0.0, 0.1]$, as, for $p_{\neq} = 0.1$ the system is at the critical value that is encountered for the regime in which both p_+ and p_{\neq} are non-zero in the sense of Sec. 3.5.2, ($p_+ \neq 0, p_{\neq} \neq 0$): $p_+^c \approx 0.2488$. In Fig. 3.12 we also show

a fit to the data, which is of the form

$$p_+^c(p_-, p_\neq \rightarrow 0) = \frac{1}{(u + v p_\neq)} + t. \quad (3.73)$$

The fit parameters were found to be

$$u = 34.6 \pm 0.3 \quad (3.74)$$

$$v = 1823 \pm 72 \quad (3.75)$$

$$t = 0.2462 \pm 0.0003. \quad (3.76)$$

It has to be noted that this formula only stands on empirical grounds, fits by exponential functions may also be useful.

3.6.2 $p_- \rightarrow 0$ Limit

Again, for completeness, we also want to discuss the second possible limit where one of the bond types is disabled. We thus set p_- to some fixed value $p_- \in [0, 1]$ and then subject p_\neq to a variation with the nested interval method algorithm in order to find its critical value p_\neq^c . Again, having determined p_\neq^c , we calculate the corresponding p_+^c and then show p_+^c versus the bond existence probability p_- . This has been done in Fig. 3.13. The curve does not look any different from the one displayed in Fig. 3.13 and a fitting procedure with the function given in (3.73) reveals the following fit parameters, which are in very good accordance with (3.74).

$$u = 33.7 \pm 0.3 \quad (3.77)$$

$$v = 1744 \pm 73 \quad (3.78)$$

$$t = 0.2461 \pm 0.0003 \quad (3.79)$$

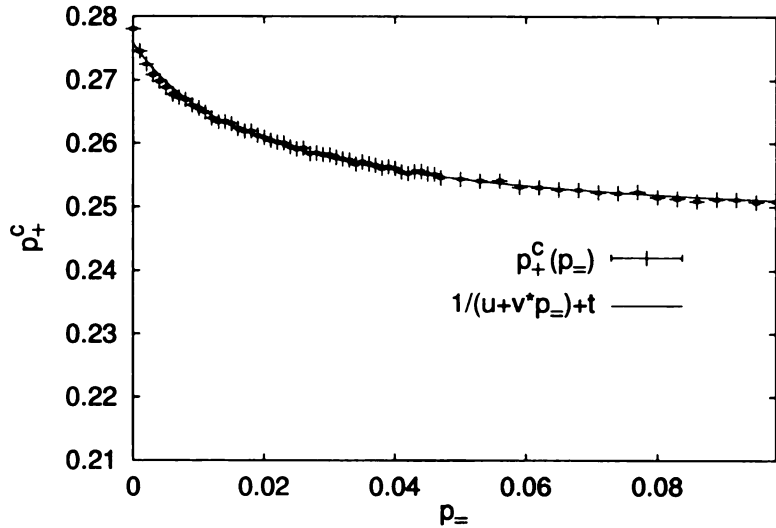


Figure 3.13: Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.5$, plotted as a function of p_- .

3.6.3 Concentration Dependence in the $p_{\neq} = 0$ Limit

In the preceding section we showed the behavior of the system for either one of the bond probabilities going to zero. We observed that the critical value of the scaled control variable, p_+ under goes a continuous phase transition when letting $p_- \rightarrow 0$ or $p_{\neq} \rightarrow 0$. Until now, in this question of the limiting behavior we have only been looking at a system with a fixed concentration of blue species of $f_b = 0.5$. We can presume that for values of the blue species concentration $f_b \neq 0.5$ the general behavior of a continuous transition will be conserved. This indeed is true, as simulation results indicate, as shown in Fig. 3.14. Also shown is a fit to the data, as in (3.73) of the form

$$p_+^c(p_-, p_{\neq} \rightarrow 0) = \frac{1}{(u + v p_{\neq})} + t, \quad (3.80)$$

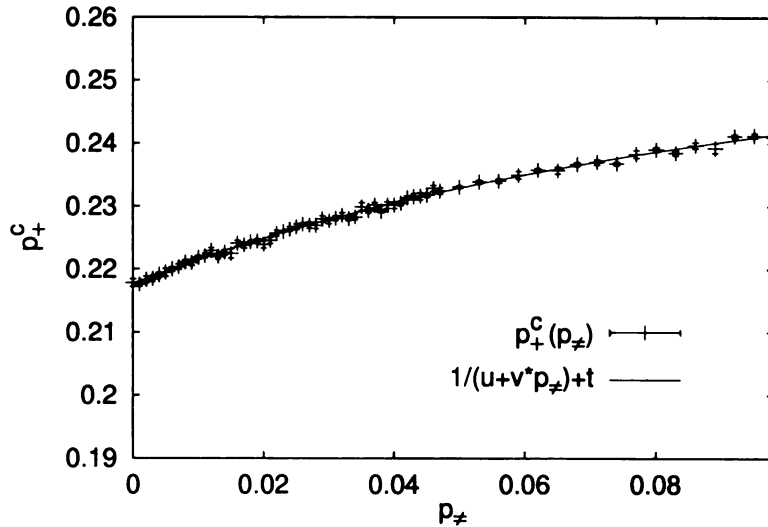


Figure 3.14: Critical value of the scaled control parameter, p_+^c , in a 128^3 simple cubic lattice with $f_b = 0.3$, plotted as a function of $p_≠$.

where the fit parameters were found to be

$$u = -17.6 \pm 0.7 \quad (3.81)$$

$$v = -129.0 \pm 14.6 \quad (3.82)$$

$$t = 0.274 \pm 0.003 \quad (3.83)$$

in this case. It can be seen that the limiting value of $p_+^c(p_≠ = 0)$ is not the same as for $f_b = 0.5$ and we suspect a concentration dependence of the threshold in the limit $p_≠ \rightarrow 0$. We undertook simulations, again of simple cubic lattices of size $L = 16^3$, $L = 32^3$, $L = 64^3$ and $L = 128^3$, at different concentrations of the blue species, determining the critical value of the bond density for $p_≠ = 0$. The results shown in Fig. 3.15 are fits of the data obtained from the simulations on the four different lattice sizes to the scaling law given in Sec. 2.5 in (2.89):

$$|p_+^c(L) - p_+^c| \propto L^{-1/\nu}, \quad (3.84)$$

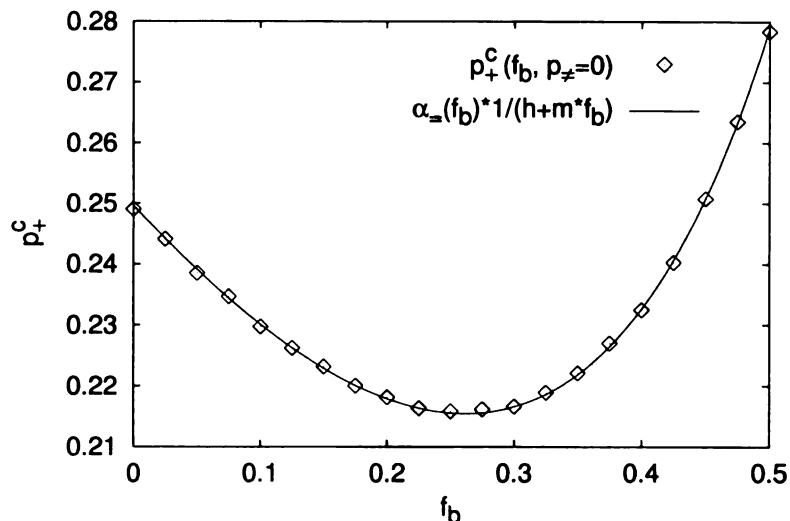


Figure 3.15: Critical value of the scaled control parameter, p_+^c , plotted as a function of the fraction of blue sites, f_b , in the limit $p_\neq = 0$ and obtained from simulations on simple cubic lattices of size $L = 16^3$, $L = 32^3$, $L = 64^3$ and $L = 128^3$ by a fit to the scaling law $|p_+^c(L) - p_+^c| \propto L^{-1/\nu}$. The errors, estimated as described in [vdM97], are smaller than the symbol sizes.

where by p_+^c we mean to indicate the threshold in a lattice of infinite extent. The critical exponent ν was kept fixed at

$$\nu = 0.88. \quad (3.85)$$

We already alluded to the problem of the estimation of systematic errors in the context of finite size scaling. We will come back to a discussion of different estimation techniques in Sec. 3.7 and for the moment content ourselves with the statement that the estimates we performed led to errorbars smaller than the symbol size in Fig. 3.15.

Also shown in Fig. 3.15 is a fit of the data with

$$p_+^c(f_b, p_\neq = 0) = \frac{2(f_b - \frac{1}{2})^2 + \frac{1}{2}}{h + mf_b}. \quad (3.86)$$

This is Eq. (3.13) for the critical values with the purely empirical assumption of a hyperbola for $p_-^c(f_b)$, which is in agreement with the results of Heermann and Stauffer for a one component site-bond model [HS81]. Fitting the parameters to our

simulation data results in

$$h = 4.007 \pm 0.002 \quad (3.87)$$

$$m = -4.428 \pm 0.005 \quad (3.88)$$

A comparison with the formula given by Heermann and Stauffer yields

$$\begin{aligned} h &= \frac{1}{p_{bond}^c} \\ &= 4.019 \end{aligned} \quad (3.89)$$

$$\begin{aligned} m &= \frac{1 - p_{bond}^c}{p_{bond}^c(f_{site}^c - 1)} \\ &= -4.386, \end{aligned} \quad (3.90)$$

where $p_{bond}^c = 0.2488$ and $f_{site}^c = 0.3116$ are the percolation thresholds for one component bond- and site- percolation on a three dimensional simple cubic lattice, respectively. However, in contrast to the one component model, due to the symmetry introduced in the system, notably that $p_{=} \equiv p_{bb} = p_{rr}$, see (3.10) in Sec. 3.2.1 we only have $f_b \in [0.0, 0.5]$ as independent regime here, with the interval $f_b \in [0.5, 1.0]$ being symmetric to the one shown here, with only the roles of blue and red sites being switched. This is a manifestation of the two components behaving like two superposed, non-interfering one component site-bond percolation systems. We further illustrate this interpretation in the following. We presume that in the limit we are discussing right now, $p_{\neq} = 0$, there is no cross influence from the two species. We check this presumption by taking the empirical formula as shown above or as given in [HS81] for a one component site-bond percolation model and plotting them for a concentration f_b and a concentration $f_r = (1 - f_b)$. This corresponds to an isolated system of blue sites with concentration f_b and a second isolated system of red sites with concentration $f_r = (1 - f_b)$ and yields Fig. 3.16. For ease of comparison, we express both concentrations in terms of one and thus for both curves do we use the

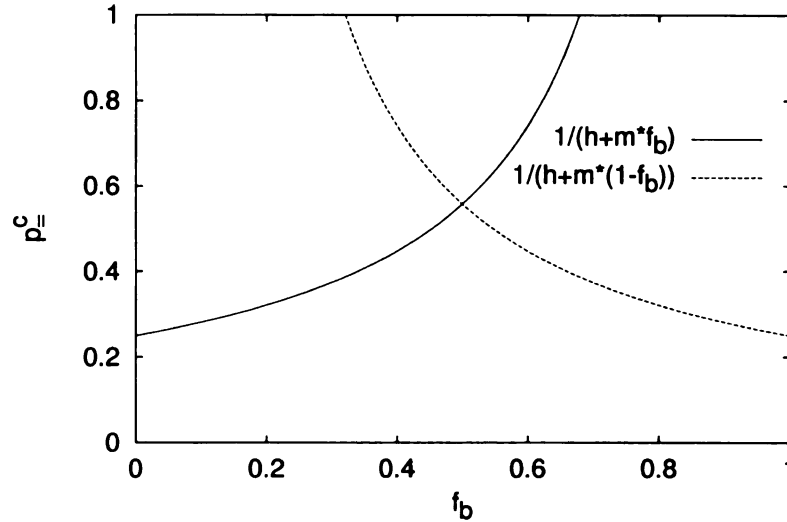


Figure 3.16: Threshold p_{\pm}^c versus concentration f_b for two one-component site-bond percolation models.

same variable f_b . Following the presumption that both behave independently, we just consider the two curves as superposed and obtain a phase diagram for the two component system, by regarding the left axis as showing p_{\pm} and not its critical value p_{\pm}^c . We first realize that indeed we do reproduce a picture with a symmetry with respect to $f_b = 0.5$ and secondly that there are three phases:

1. Below both curves: No percolation.
2. Above one of the curves, below the second: One component percolates.
3. Above both curves: Both components percolate.

We can also transform the natural variable that we have used so far in the analysis, p_{\pm}^c to the scaled control variable p_{\pm}^c . We show the phase diagram in terms of p_{\pm}^c in Fig. 3.17. The curves now are in the same shape as our simulation results. We can summarize two facts: First the fact that indeed in the limit $p_{\neq} = 0$ the two-component site-bond percolation system may be described by two superposed, independent one component site-bond percolation systems and second that the two-component site-

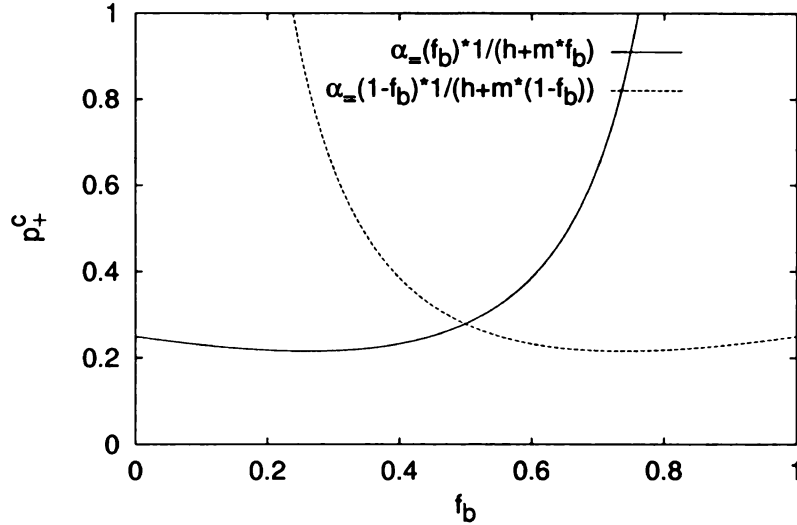


Figure 3.17: Threshold p_+^c versus concentration f_b for two one-component site-bond percolation models.

bond percolation system essentially behaves as a one-component bond-percolation system when both bond types are active, see Sec. 3.4.1. These two facts let us conclude that the phase transition in p_+^c observed for $p_- \rightarrow 0$, see Sec. 3.6.1, may be interpreted as an effective transition from a one-component bond percolation model to a one-component site-bond percolation model.

3.6.4 The Cut-Out Technique

In addition to the confirmation of the finding (3.86) through the results of Heermann and Stauffer, we also performed another type of simulation to check on the decreasing behavior of p_+^c in the regime for small f_b . It has to be stated that this method does not represent a thorough verification, however it does give a good confirmation of the results. We simulated a one-component bond percolation system on a simple cubic lattice at some fixed $p_- > p_-^c$, let the cluster structure evolve and then determined the percolation probability. In a second step an algorithm swept through the whole lattice, cutting out sites at random with a given probability p_{cut} , which was varied,

$p_{cut} \in [0, 1]$, and determined the percolation probability again. In Fig. 3.18 we show the percolation probability p_∞ as a function of the probability that an arbitrary site gets cut out, p_{cut} . A linear, decreasing dependence on the cut-probability is observed

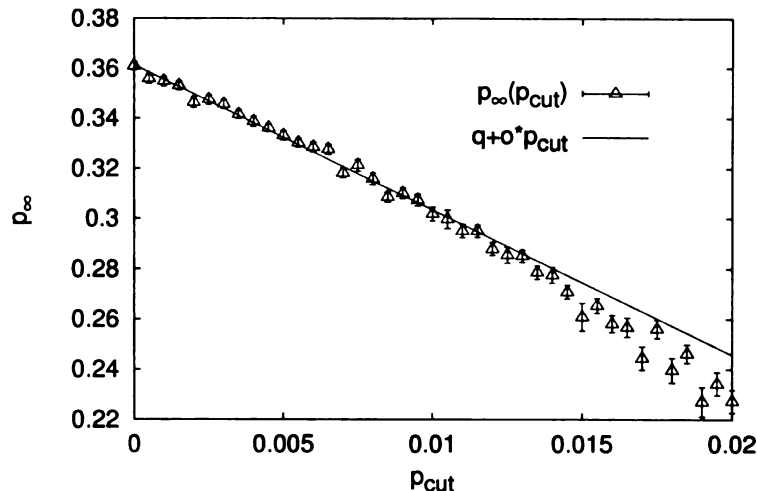


Figure 3.18: Percolation probability p_∞ versus the probability that a site gets 'cut-out', p_{cut} .

in the first regime, for $p_{cut} \gtrsim 0.012$ a stronger decrease sets in. For completeness, we state the values of the fit parameters for the linear fit

$$p_\infty(p_{cut}) = q + o p_{cut}, \quad (3.91)$$

of the data also shown in Fig 3.18, which are

$$q = 0.361 \pm 0.001 \quad (3.92)$$

$$o = -5.8 \pm 0.1. \quad (3.93)$$

We can relate p_{cut} to f_b and through the observation of a decreasing p_∞ can make plausible a linear rise of p_-^c with p_{cut} or. In the framework of the two-component model in the $p_\neq = 0$ limit, p_{cut} corresponds to f_b . In the same regime however, we have a quadratically decreasing function $\alpha_=(f_b)$, see Fig. 3.7. To arrive at the threshold p_+^c , we have to multiply p_-^c with $\alpha_=(f_b)$, which then will be decreasing, dominated by

the quadratic decrease in $\alpha_{=}$. It has to be noted that the argument is only valid for relatively small values of the cutout probability p_{cut} since at higher values the system shows a rapid decrease to a vanishing percolation probability. It is at least an intuitive, heuristic argument for explaining the seemingly counter-intuitive effect of a decreasing threshold with an increasing number of sites of another species, which in the limit p_{\neq} act as geometrical obstructions for the percolating major concentration species. We have to emphasize again that this is by far no thorough argument but rather one of mere plausibility, giving however a good intuitive explanation for the decrease of p_{+}^c for small f_b .

3.6.5 Concentration Dependence in the $p_{=} = 0$ Limit

We now come to the question of the concentration dependence in the case where all edges connecting sites occupied by the same species are closed always. In the preceding sections we found that the percolation probability does not show a different behavior whether $p_{\neq} \rightarrow 0$ or $p_{=} \rightarrow 0$. Here however, it will become clear, that contrary to the percolation probability, the critical value of the bond density, p_{+}^c , does show a different behavior in the two different limits. The simulation is essentially the same as described in Sec. 3.6.3, $p_{=} = 0$ is set and with the nested interval method the critical value of p_{\neq} is determined, from which p_{+}^c is calculated. Again we undertook simulations on simple cubic lattices of size $L = 16^3$, $L = 32^3$, $L = 64^3$ and $L = 128^3$ and then fitted the results with the scaling relation (3.84), providing us with the 'true' threshold in the limit of the lattice size $L \rightarrow \infty$. The same discussion as led in Sec. 3.6.5, concerning the systematic errors, applies and again we refer to Sec. 3.7 for a more complete discussion. We present the simulation results in Fig. 3.19. In the upper curve of Fig. 3.19 we go back to the bond existence probability p_{\neq} . Its critical value, as a function of the concentration, $p_{\neq}^c(f_b)$, is well reproduced with an

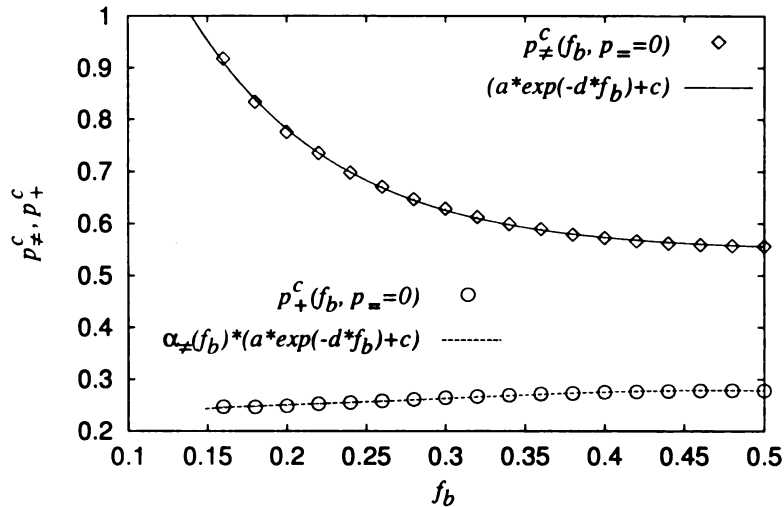


Figure 3.19: Critical value of p_{\neq} and of the scaled control parameter, p_{\neq}^c and p_+^c , plotted as a function of the fraction of blue sites f_b in the limit $p_{=} = 0$. The data has been obtained by a fit to $|p_+^c(L) - p_+^c| \propto L^{-1/\nu}$. Again the errors, estimated as described in [vdM97], are smaller than the symbol sizes.

exponential fit:

$$\begin{aligned} \varphi &= p_{\neq}^c(f_b) \\ &= a \exp(-d f_b) + c \end{aligned} \quad (3.94)$$

Fitting this empirical formula to the simulation data gives

$$a = 2.1 \pm 0.07 \quad (3.95)$$

$$d = 10.9 \pm 0.2 \quad (3.96)$$

$$c = 0.547 \pm 0.002 \quad (3.97)$$

We define

$$f_b^c \equiv \varphi^{-1}(p_{\neq}=1) \quad (3.98)$$

and numerically get

$$f_b^c \simeq 0.14 \quad (3.99)$$

fre

as

of

wh

L

si

a

s

w

i

h

n

from (3.94). We then also conduct an independent simulation, making use this time, as described in Sec. 3.3, of the nested interval method to determine the critical value of f_b . We find

$$f_b^c = 0.145 \pm 0.001, \quad (3.100)$$

which again is a result from a fit with data obtained on simple cubic lattices of size $L = 16^3$, $L = 32^3$, $L = 64^3$ and $L = 128^3$ to the scaling relation (3.84). What is the significance of the parameter f_b^c ? Let us first consider the inverse case, where $p_{\neq} = 0$ and $p_{=} = 1$. In this limit we effectively deal with a one-component site percolation system, since one bond type is entirely 'switched off' and the other edges are open with probability one. This implies that we can decide to call one component the inactive one, say the red species, and focus on the second species. If two blue sites have one edge in common, it is open with probability one. This however, is exactly the rule in a one-component site percolation system where the site percolation threshold is known to be $f_{site}^c = 0.3116$, (3.42), for a simple cubic lattice. In the exactly inverse case, ($p_{=} = 0, p_{\neq} = 1$), if two vertices occupied by different species have one edge in common, it is open always. We thus conclude that f_b^c can be regarded as a new site percolation threshold in a simple site percolation system in which, unlike the ordinary site percolation model, nearest neighbors only belong to the same cluster if they are of opposite flavor. In the lower curve of Fig. 3.19 we show the critical value of the bond density, p_+^c . It is simply given as the product of $p_{\neq}^c(f_b)$ with the edge density $\alpha_{\neq}(f_b)$, see (3.13) and (3.14):

$$\begin{aligned} p_+^c(f_b, p_{=} = 0) &= \alpha_{\neq}(f_b) p_{\neq}^c(f_b) \\ &= \left(\frac{1}{2} - 2(f_b - \frac{1}{2})^2 \right) (a \exp(-d f_b) + c) \end{aligned} \quad (3.101)$$

Here, f_b^c determines the critical point of the phase transition line $p_+^c(f_b, p_{=} = 0)$. An argument against a novel behavior could be the statement that in this case, the

concentration of one species is no longer the appropriate parameter to characterize the state of the system. To show that this argument does not hold for this purpose, we propose one such new parameter that should be universal for the percolation systems dealt with in this work. This is the *density of accessible edges*, which was already introduced in (3.7), or, more specifically, for a two-component model in (3.14) and (3.15). Although usually edges are not included as ingredients in a site percolation system, this quantity makes sense for a site percolation system too, as edges are readily included in the line of argument of a site percolation system by setting them open with probability one. For the model considered here the density of accessible edges is given by $\alpha_{\neq}(f_b)$ and at the new critical site percolation threshold f_b^c we have

$$\alpha_{\neq}^c(f_b^c) = \frac{1}{2} - 2\left(f_b^c - \frac{1}{2}\right)^2. \quad (3.102)$$

For the ordinary site percolation system in which neighbors of the same flavor form clusters, we have the density of accessible edges given as

$$\alpha_{site} = (f_{site})^2, \quad (3.103)$$

and the critical value

$$\alpha_{site}^c = (f_{site}^c)^2. \quad (3.104)$$

Then, if both systems were equal with respect to this variable, the critical density of accessible edges in both systems would be expected to be the same:

$$\alpha_{\neq}^c \equiv \alpha_{site}^c. \quad (3.105)$$

This requires

$$f_b^c = \frac{1}{2} \mp \frac{1}{2} \sqrt{1 - 2\alpha_{site}^c}, \quad (3.106)$$

giving two solutions, symmetric with respect to $f_b = 0.5$,

$$f_b^c = 0.051, \quad (3.107)$$

an

T

an

3

In

T

es

a

a

3

I

(

I

f

t

c

r

|

and

$$f_b^c = 0.949. \quad (3.108)$$

This stands in obvious contradiction to our findings. We conclude that this is another argument in favor of a qualitatively new behavior.

3.7 Finite Size Effects

In the preceding sections we alluded several times to the subject of error estimates. The statistical errors are not the ones that are troublesome, how a reasonably precise estimate of the systematic errors resulting from finite size effects can be achieved, is a more complicated subject. We will first focus on the one-dimensional case again and then discuss briefly techniques that we used.

3.7.1 One-Dimensional Percolation Model

In Sec. 2.5 we derived the finite size scaling law for one dimensional percolation, see (2.82) which read

$$p_c - p_{\text{eff}} \propto L^{-1/\nu}. \quad (3.109)$$

In the derivation we stated that it would be necessary to fulfill the condition

$$|p - p_c| \ll 1.$$

for the scaling law in the approximative form, as derived, to be valid. We now want to know, how big the systematic errors are when we apply the scaling law to lattices of small linear dimension. Why are systematic errors to be expected at all? The reason lies exactly in the fact that in the derivation in Sec. 2.5 the approximation $|p - p_c| \ll 1$ was used. This led to the relatively simple expression of

$$p_{\text{eff}}^{\text{approx}} = 1 - \frac{1}{L}.$$

Had we not used this approximation, we would have obtained

$$p_{eff}^{exact} = \exp(-1/L), \quad (3.110)$$

resulting from

$$\Pi(p_{eff}) = 1/e,$$

see (2.79). By relying on the approximative formula, however, the necessary condition for its validity can not be satisfied any more, since for small L the system is not close to the threshold. We therefore implicitly also have the condition

$$\frac{1}{L} \ll 1. \quad (3.111)$$

The systematic error entering the finite size scaling can be readily calculated,

$$\begin{aligned} \sigma_{sys} &= \left| \exp(-1/L) - 1 + \frac{1}{L} \right| \\ &= \sum_{n=2}^{\infty} \frac{-L^{-n}}{n!}. \end{aligned} \quad (3.112)$$

We illustrate this effect in Fig. 3.20. In the next section we will go to a discussion of the same phenomenon in higher dimensions, where it will become clear that the analytical treatment presented here in the case of one dimension will not be possible any more and one has to rely on estimation techniques.

3.7.2 Techniques in Higher Dimensions

In Sec. 2.5 we had conjectured a certain scaling behavior, (2.84) and from that derived the scaling relation (2.89). In both equations, it was a requirement that

$$|p_{eff}(L) - p_c| \ll 1 \quad \text{and} \quad L \gg 1.$$

It is the second condition that one has to worry about. It is not a priori clear where the linear dimension L of a lattice has to lie in order to be able to neglect the errors

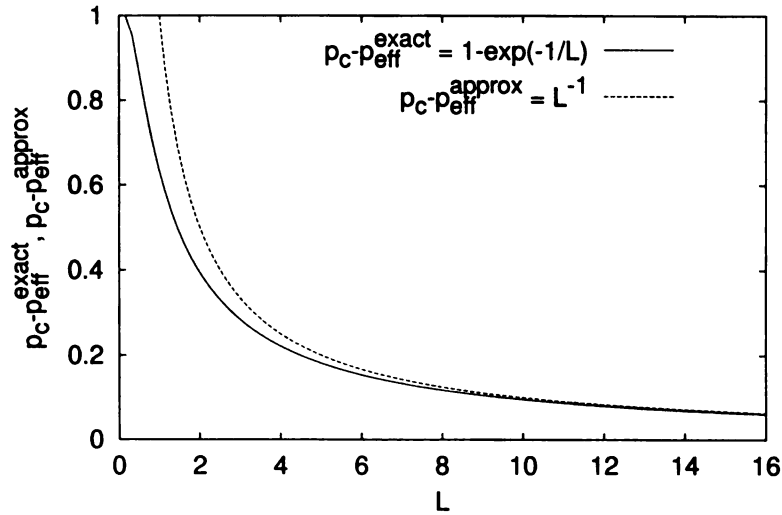


Figure 3.20: Exact (solid line) and approximative (dashed line) effective threshold in a one-dimensional percolation system as a function of the linear lattice dimension L .

that are due to applying the finite size scaling equation in a regime where it only holds in a very approximative way. We want to illustrate the situation that one faces when applying the finite size scaling relation, (2.89), in Fig. 3.21, in which we show the critical value of the bond density, p_+^c , as a function of the linear lattice dimension, as well as a fit with

$$|p_+^c(L) - p_+^c| = a L^{-1/\nu}. \quad (3.113)$$

What is the 'true' value of p_+^c ? One way to proceed is to fit the data with (3.113). The true threshold is obtained as a fit parameter, together with an error estimate. Another possibility constitutes of plotting the data in a double logarithmic plot and then fitting with p_+^c as fit parameter such that the expectation of a straight line

$$\ln |p_+^c(L) - p_+^c| = \ln a - \frac{1}{\nu} \ln L, \quad (3.114)$$

where $a = \text{const}$, is fulfilled. This would also provide an error estimate for the fit parameters. We applied the first method, as shown in Fig. 3.21. This led to errorbars smaller than the symbol size in Fig. 3.15. We have to note that this method does not

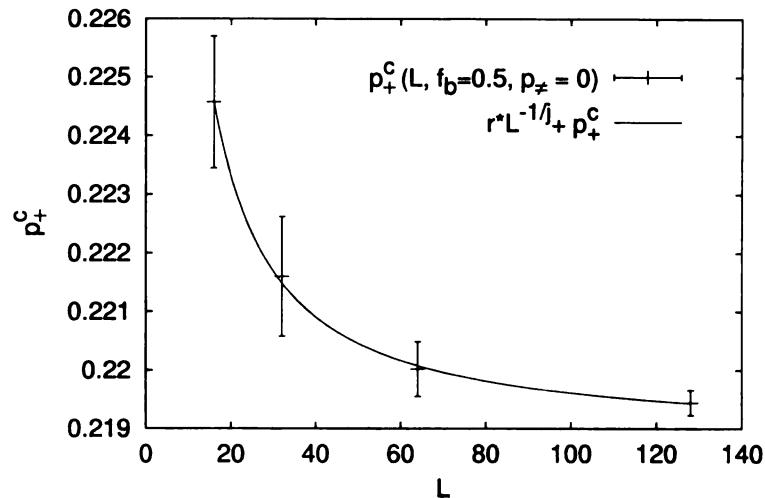


Figure 3.21: Finite size scaling for $p_+^c(L, p_x = 0)$ shown as a function of the linear dimension of a simple cubic lattice at a concentration of the blue species of $f_b = 0.5$.

explicitly provide for an estimate of the systematic errors themselves. This is, as the only weighting of the data points used in the fitting procedure comes in through the statistical errors attached to each data point, no weighting that takes into account the 'distance' from the validity region of the scaling law is included. On the other hand, the statistical errors do show a finite size scaling: The errorbars for smaller lattice sizes turn out to be bigger than those for larger lattices, see Fig. 3.21, even though the same number of events has been taken into account for calculating the averages and their errors. Thus we already include a systematic finite size error in the procedure. Yet this should not account for the second kind of systematic errors, the ones due to the application of (3.113), which is only valid for $L \rightarrow \infty$. Is there a way to estimate the errors solely due to the finite size scaling law? One way that we can think of, is to try to find a sort of a finite size weighting factor scaling for the error influence of each data point in a finite size scaling procedure. This scaling function could, for example be in the form of an exponential.

A search of the literature did not reveal any thorough discussion on an estimate

of the systematic errors in a determination of the 'true' threshold $p_+^c(\infty)$ due to finite size scaling. We found two ways of dealing with the systematic error, where one method tries to estimate them and the second tries to avoid them in the calculation of the true threshold. We will present both methods.

The first method was proposed in [vdM97]. It relies essentially on fitting the data with (3.113). The thresholds are calculated for different lattice sizes. Two fits are done, one including the last three data points, giving $p_+^c(L_{max}, L_{max-1}, L_{max-2})$ the other including the last two data points resulting in $p_+^c(L_{max}, L_{max-1})$. The difference between the two fit parameters is then taken as estimate for the systematic error,

$$\sigma_{sys} = \left| p_+^c(L_{max}, L_{max-1}, L_{max-2}) - p_+^c(L_{max}, L_{max-1}) \right|. \quad (3.115)$$

We also performed calculations following this method to estimate the systematic errors. Again, the errorbars obtained were smaller than the symbol size in Fig. 3.15. A way to implement essentially this same method in what might be an improved way would be to do the finite size scaling for all combinations of available data points, not only fitting the last two and the last three, and then taking the largest difference between the resulting fits for p_+^c as estimate for the error σ_{sys} .

The second method is described in [BH97]. In this case, not the percolation probability p_∞ but rather the probability that a cluster spans the entire system, ψ , is taken to be the observable. For the infinite lattice, we have

$$\psi = \begin{cases} 0, & \text{if } p \leq p_+^c \\ 1, & \text{if } p > p_+^c \end{cases}. \quad (3.116)$$

As a consequence, all $\psi_L(p_+)$ have a common intersection point $\psi_{L_{max}}(p_+^c)$, which we illustrate in Fig. 3.22. Extrapolation to $L_{max} \rightarrow \infty$ yields an estimate for the percolation threshold p_+^c . The advantage of this method is that it does not involve the choice of a critical exponent, as ν in (3.113). Furthermore it does not involve a scaling

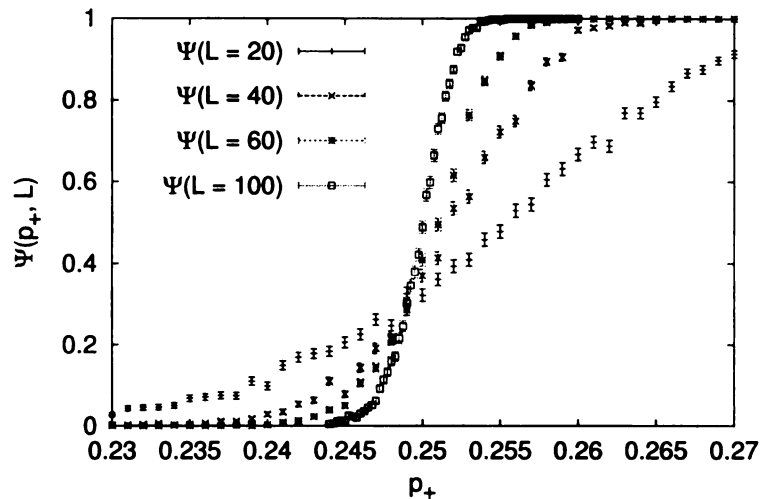


Figure 3.22: Probability ψ that a spanning cluster exists, versus the lattice size L . The percolation threshold p_+^c is given by the common intersection point $\psi_{L_{max}}(p_+^c)$.

relation. However, still an extrapolation to $L \rightarrow \infty$ is needed and the determination of the percolation threshold itself is not without error.

3.7.3 A Proposal for a Novel Technique

In Sec. 3.3.3 we described the approach that we took to determine, in a simulation, the critical values p_-^c , p_+^c and f_b^c . In summary, the simulation first carried out the nested interval method and thus determined the threshold for one particular random number sequence, then the algorithm was started with another random number sequence and after a sufficient number of independent simulations, the average gave the critical value. Another way to proceed, however, would be to just do the inverse: First carry out many independent simulations, determine the percolation probability or the spanning probability and then, decide, according to an appropriately chosen value a , whether the system percolates or not. The parameter a could be chosen such as to give an effective threshold of $1/e$, for example, as in (2.79), or, in general,

$$p_{eff} = \psi^{-1}(a). \quad (3.117)$$

Based on this averaged information, whether $p_\infty < a$ or $p_\infty > a$, the decision about the nested interval method would be made and the new 'test' value for the parameter p_+ , p_\neq or f_b chosen, at which again a number of independent simulations would yield the decision about the further direction of the parameter value. How does one obtain a way to estimate the systematic errors when applying this method? The idea is to apply the same procedure to several values of a and furthermore at different lattice sizes L , where three different lattice sizes would be a minimum requirement. Another requirement is the knowledge of an interval Δp_+^i for which, from theoretical considerations, we know definitely

$$p_+^c \in \Delta p_+. \quad (3.118)$$

p_+^c denotes the 'real' threshold in a system of infinite extent. Through ψ this interval Δp_+^i gets mapped onto an interval of values a , Δa_i . We would then get three different curves: $p_+^c(\Delta a_1^i, L_1)$, $p_+^c(\Delta a_2^i, L_2)$ and $p_+^c(\Delta a_3^i, L_3)$. In the following the finite size scaling law should be applied to all combinations of points

$$\{p_+^c(b_1, L_1), p_+^c(b_2, L_2), p_+^c(b_3, L_3)\} \quad (3.119)$$

with the condition that

$$b_1 \in \Delta a_1^i, \quad b_2 \in \Delta a_2^i, \quad b_3 \in \Delta a_3^i, \quad (3.120)$$

where the case of a higher number of lattice sizes to take into consideration, works in an analogous way. This eventually leads to a hyperplane

$$p_+^c(b_1, b_2, b_3, L \rightarrow \infty). \quad (3.121)$$

Now the minimum $p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{min}^i$ and maximum $p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{max}^i$ have to be determined, giving an estimate of the error,

$$\sigma_{sys} = |p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{min}^i - p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{max}^i|, \quad (3.122)$$

and, as average taken over the hyperplane, the critical value p_+^c . The interval

$$\Delta p_+^{i+1} = [p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{min}^i, p_+^c(b_1, b_2, b_3, L \rightarrow \infty)_{max}^i], \quad (3.123)$$

may be taken as new input in the procedure and in successive iterations the critical value will be known with an error estimate. This method is based on ideas of von Bergmann [vB99] and has evolved in several discussions with the author. It has to be noted however that its practical aspects could not yet be tested and thus it remains unclear whether it can live up to the expectations when applied to the determination of the threshold and an estimate of its error.

3.8 Spin-Off Results

In this section, we will present some topics and related results that were not the main interest in the line of research, but yet, in the pursuit of the main objectives, were investigated in the line of work. We will not give a broad discussion of each of the results but rather summarize in a concise manner the main aspects.

3.8.1 The Number of Open Clusters per Vertex

We already introduced the number of open clusters per vertex in Sec. 2.4.3. The programs used determined this quantity that has also been called the *f-function* and we show a result for two different values of the concentration of the blue species in Fig. 3.23. Also shown in the figure is the theoretical expectation, which we derive in the following way, see [Bau]. The total number of open clusters per vertex has to be calculated as given in (2.32). The first terms of this sum can still be given analytically, we consider the first two:

$$\begin{aligned} \kappa(p_+) &= N(1 - p_+)^z + \frac{Nz}{2} p_+ (1 - p_+)^{2z-2} + \dots \\ &= N(1 - \frac{z}{2} p_+) + \mathcal{O}(p_+^2). \end{aligned} \quad (3.124)$$

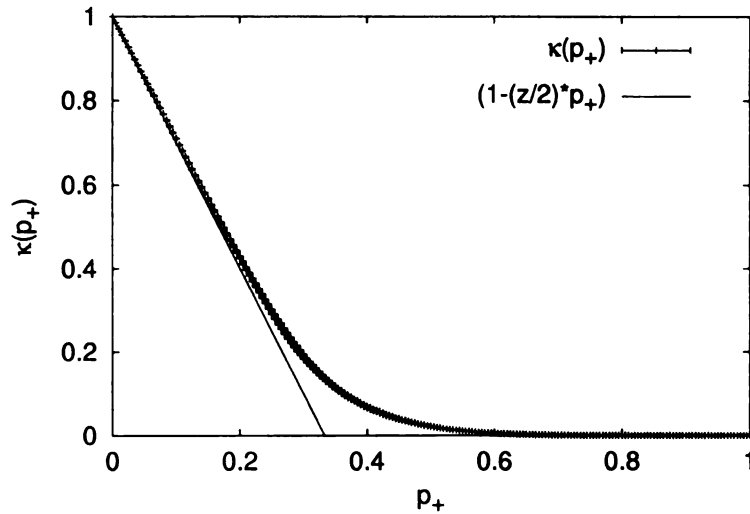


Figure 3.23: The number of open clusters per vertex in a simple cubic 128^3 lattice, calculated for a concentration of the blue species $f_b = 0.5$. Also shown is the approximate theoretical expectation.

Here, N is the total number of vertices in the lattice,

$$N = L^3,$$

and z is the coordination number of the lattice type, thus $z = 6$ in our case of the simple cubic lattice. In Fig. 3.23 we see that indeed this approximation, which, because of the expansion made in the derivation is valid for $p_+ \ll 1$, does hold in this regime. Finite size effects are not taken into account here. Thus we find exactly what is to be expected: For low values of p_+ the lattice is highly fragmented, showing a high number of small clusters, whereas for high values of p_+ gradually larger clusters take over.

3.8.2 The Number of Spanning Clusters per Vertex

For the infinite lattice, according to Theorem 1, there can almost always be only one infinite cluster present in the lattice and this will be the largest cluster. For finite lattices however, a finite probability exists that more than one cluster spans

the entire system. Furthermore, also a finite probability exists for a smaller cluster than the largest one to percolate. The question is, whether this affects the percolation threshold in a finite lattice, and if it does, in which way. In an attempt to estimate the influence of this finite size effect on the percolation probability p_∞ , we introduced a new quantity, which we called p_{pc} and which represents the probability that an arbitrary vertex of the lattice is part of any of the percolating clusters. If there is only one percolating cluster, then we have p_∞ and p_{pc} equal. Thus, as we have the theorem on the uniqueness of the infinite cluster in the limit of an infinite system, we know that

$$\lim_{L \rightarrow \infty} p_\infty = \lim_{L \rightarrow \infty} p_{pc}. \quad (3.125)$$

We tested the new order parameter for several lattice sizes and focused on the question of a difference in the percolation thresholds in terms of both variables. Within the limits of the errorbars we could detect no different behavior, indicating that the definition of the infinite cluster in a finite system and the checking mechanisms for it, see (2.10) and (2.11) are reasonable. We show one such comparison of p_∞ and p_{pc} in Fig. 3.24. Analogously to p_{pc} we can also define a 'new' spanning probability, given as the probability that any cluster, not necessarily the one that complies with the requirements for being the infinite cluster, C_∞ , percolates. We denote this quantity by ψ_{pc} . Similarly to the results shown above, no difference in the percolation thresholds derived from ψ or ψ_{pc} , could be detected. With the theorem of the uniqueness of the infinite cluster we again have

$$\lim_{L \rightarrow \infty} \psi = \lim_{L \rightarrow \infty} \psi_{pc}. \quad (3.126)$$

With these two results it is confirmed that the percolation probability as used by us in the framework of the research presented here in order to determine the percolation threshold, is a sensible observable.

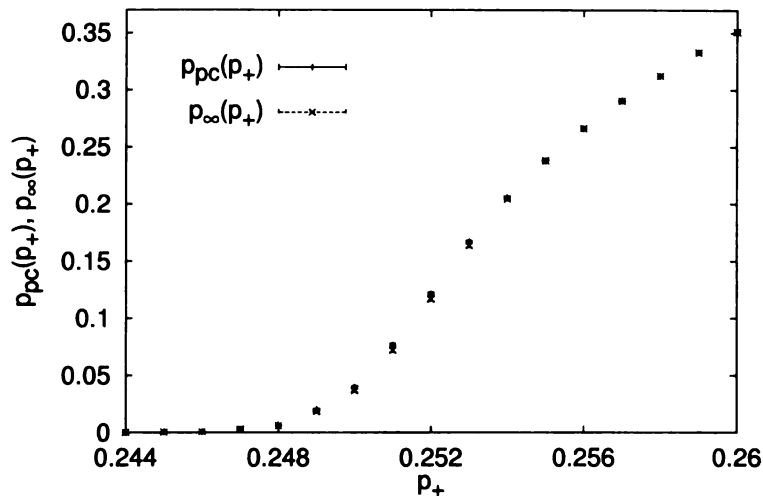


Figure 3.24: Probability to belong to the infinite cluster, $p_{\infty}(p_+)$, and the probability to belong to any percolating cluster, $p_{pc}(p_+)$ in a simple cubic 100^3 lattice at $f_b = 0.5$.

3.8.3 Two-Dimensional Percolation

In Sec. 2.2.4 we discussed that in general critical exponents are expected to be universal, meaning that they only depend on the dimension of the system, but not its microscopic structure. The critical exponents for two dimensional ordinary bond percolation problems are well known, see for example, [SA94]. Obviously the question remains to be answered whether the results presented in this work for two-component site-bond percolation on a three dimensional simple cubic lattice do in principle hold on a two dimensional lattice too. We investigated this question in some aspects on a square lattice. More specifically we focused on the question of the concentration dependence of the threshold in the limits of one of the two bond existence probabilities set to zero: $p_- = 0$ or $p_{\neq} = 0$, see 3.6.3 and 3.6.5. Before we proceed to state the results we have to note that there is a fundamental difference concerning two-component site-bond percolation on a simple cubic lattice and two-component site-bond percolation on a square lattice. This difference lies in the fact that on the simple cubic lattice a panchromatic regime does exist, which is not the case for the square

lattice. This comes about as the site percolation threshold on the square lattice is noticeably higher than on the simple cubic lattice, leading to non-overlapping curves. We illustrate our statement with Fig. 3.25 and also want to refer to Sec. 3.6.3, where we led the corresponding discussion for the simple cubic lattice. Fig. 3.25 essentially is Fig. 3.16 for the square lattice. We take again the assumption of a hyperbola, see

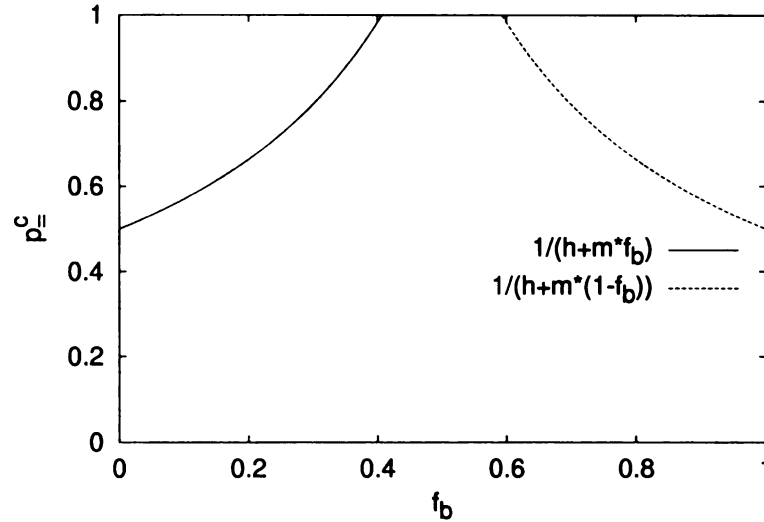


Figure 3.25: Threshold $p_c^=$ versus concentration f_b for two one-component site-bond percolation models on the square lattice, compare Fig. 3.16.

(3.86),

$$p_c^=(f_b, p_{\neq} = 0) = \frac{1}{h + m f_b}. \quad (3.127)$$

This is justified by simulations performed by us, results of which could very well be reproduced by a hyperbola of the given form with the parameters as calculated in (3.128). We calculate the parameters as in (3.89), with $p_{bond}^c = 0.5$ (exact, see [SE64])

and $f_{site}^c = 0.5927$ for the square lattice yielding

$$\begin{aligned} h &= \frac{1}{p_{bond}^c} \\ &= 2 \end{aligned} \tag{3.128}$$

$$\begin{aligned} m &= \frac{1 - p_{bond}^c}{p_{bond}^c(f_{site}^c - 1)} \\ &= -2.455. \end{aligned} \tag{3.129}$$

In contrast to the curves for the simple cubic lattice it becomes clear in Fig. 3.25 that for the square lattice, due to the higher site percolation threshold f_{site}^c , there are only two phases present, no polychromatic regime is encountered where both species percolate at the same time. Although this is no principle constraint in the sense that yet mixed clusters are possible and thus also the limiting behavior of the system when one of the bond existence probabilities is let to zero, should be investigable, we did not further involve in research in two dimensions, aside from also checking the cut-out technique, see 3.6.4, which yielded qualitatively the same results as on the simple cubic lattice. The problem could be remedied by modeling the system on a lattice of higher connectivity in two dimensions, where the site percolation thresholds are lower, see [SA94] or [Gri99].

Chapter 4

Summary and Conclusion

Since its first introduction in the context of polymer science, percolation theory has evolved to an important field, providing possibilities to study phase transitions in a framework relatively easy to model. In percolation theory a somewhat unusual phase transition is dealt with, since it does not involve any concept of temperature. Rather all interesting functions are purely geometric properties, like for example, the percolation probability or the spanning probability, and not thermal properties like specific heats as functions of temperatures as dealt with in the realm of thermal phase transitions. Nonetheless there is quite a deep similarity existent between thermal phase transitions and percolative phase transitions, which we already alluded to in Table 2.2. It also becomes clear when looking at the scaling laws that describe the asymptotic behavior of the respective systems close to their phase transition point. As in thermal phase transition simple power laws govern the behavior in the vicinity of the critical point and also do the critical exponents show the property of universality. This principle of universality suggests that one should be able to find the same critical exponents in real-life experiments as in computer experiments even though in the real experiments impurities and defects in the lattice will alter and modify the microscopic structure. As stated in [DZA83], metal-insulator films do indeed show the same behavior as found in computer experiments. Other possible applications of

percolation theory can be found again in [DZA83] or in [Sah94]. In addition, with these correspondences between thermal and percolative phase transitions, including universality of the critical exponents, an understanding of the percolative phase transitions, which are in some aspects easier to simulate and investigate, can help better the understanding of more complicated thermal phase transitions.

In summarizing, this work presented, after a general introduction to percolation theory and phase transitions in Chapter 2, research on a two-component site-bond percolation system. We first described a novel method to treat N-component percolation as described in [Baued] and [HB99]. This approach was then applied in Monte-Carlo simulations to a percolation model on a simple cubic lattice of various sizes for $N = 2$ components. We introduced a scaled control variable, p_+ , giving the bond density in the system under observation, being a function of the concentration of one of the species in the lattice, f_b , and the two bond existence probabilities p_+ and p_- . Here the intuitive notation p_+ means to indicate the probability for an edge to be open if the endvertices are of the same 'color' whereas the notation p_- stands for the probability of an edge with endvertices of different color to be open. In the simulations we determined the percolation probability p_∞ as a function of p_+ . We found that for a regime where either one of the bond existence probabilities is set to zero, $p_+ = 0$ or $p_- = 0$, the system shows a different phase transition behavior in the order parameter p_∞ , see 3.5. We could furthermore establish that there is a discontinuous phase transition taking place in the percolation probability p_∞ whence either $p_+ \rightarrow 0$ or $p_- \rightarrow 0$. As to the behavior of the percolation threshold p_+^c in the system we found that when both bond existence probabilities are non-zero, $p_+ \neq 0$ and $p_- \neq 0$, the critical value of the scaled control variable, p_+^c , coincides with the known percolation threshold in an ordinary one component bond-percolation system, $p_{bond}^c \approx 0.2488$, independent of the composition of the system characterized by f_b . In

any one of the limits $p_{=} = 0$ or $p_{\neq} = 0$ however, a different percolation threshold p_+^c is found which furthermore depends on the concentration of one of the components: $p_+^c(f_b)$. As described in Sec. 3.6, the functional form turns out to be different in both limits, we thus have $p_+^c(f_b, p_{=} = 0)$ and $p_+^c(f_b, p_{\neq} = 0)$. For the latter case we could report that an empirical formula given by Heermann and Stauffer [HS81] for a one-component site-bond percolation system applies in the two-component site-bond percolation model too. In the first case, however, a different behavior was found, for which we proposed a novel empirical formula. In a brief notation this is summarized by stating that for $p_{=} p_{\neq} \neq 0$ we find a behavior similar to one-component bond percolation, whereas for $p_{=} p_{\neq} = 0$ a different behavior is encountered. Aspects of the simulation techniques and related results were also discussed.

The field for future work in this area seems vast. As a first generalization one might try to apply the same method as described and applied here, to multi-component systems on lattices of higher dimension and/or higher connectivity. It should also be interesting to check on this percolation model with a 'bond discrimination' scheme built in, differentiating between different types of bonds for the percolation process. This approach should also find a broad range of possible applications. One might think of special networks, or gelation phenomena where several components are involved, which interact in special ways, as well as wetting phenomena. It should be possible to find applications where either one of the limits discussed above or a model with all types of bonds active, is applicable. Furthermore an application to stock-market simulations seems possible and is being undertaken by the authors of [HB99]. In concluding, the present work and the works it is based on show that, although percolation theory has grown to a field that much attention is devoted to, open questions, aside from still lacking proofs of widely accepted conjectures, remain, the answers of which have possibly useful applications to other fields of science.

Appendix A

Source Code

Following are the source codes of two of the programs used in the simulations. We display these two as being representative of the two general techniques used, as described in Sec. 3.3. All programs were written in FORTRAN and were compiled on different machines with different FORTRAN-compilers. The random number generator function listed at the end of the respective programs was taken from Ref. [PTVF92], as the standard random number generators provided on the platforms used showed correlations, especially for linear lattice dimensions $L = 128$. For an explanation of the algorithms and concepts used in the program we refer to Sec. 3.3.

A.1 perc_prob_00.f

The program displayed in the following is, as described in the section on simulation techniques used, 3.3, the general purpose program aimed at determining the percolation probability p_∞ , the probability that a spanning cluster exists, ψ , and the number of open clusters per vertex.

```
program perc_prob00
*   uses fortran 77 conventions
*   uses a random number generator taken from numerical recipes in
*   fortran 2nd ed.: ran1(iseed), modified to use double precision

implicit double precision (A-H,O-Z)
```

```

        call readpar(n, nevent, prob_nMin, dprob_n, nprob_n)
*-----
*   Loop over prob_n:
*-----
        prob_n = prob_nMin
        do iprob_n = 0, nprob_n
            call init(n, nevent, prob_n, iprob_n,
&                peqSt, dpeq, npeq, pneqSt, dpneq, npneq)
            pneq = pneqSt
            do ipneq = 0, npneq
                peq = peqSt
                do ipeq = 0, npeq
                    call Perc(n, nevent, prob_n, peq, pneq)
                    peq = peq + dpeq
                end do
                pneq = pneq + dpneq
            end do
            prob_n = prob_n + dprob_n
        end do
*-----
*   End Loop over prob_n:
*-----
        end
*-----
SUBROUTINE readpar(n, nevent, prob_nMin, dprob_n, nprob_n)

        implicit double precision (A-H,O-Z)

        parameter (maxn = 128)

*   input parameters:
*
        open(unit=12,file='parall.dat',status='old')
        read (12,*) n
*   = number of lattice sites in one direction
        if (n .gt. maxn) then
            print *, ' > Fatal Error: n must be less or equal maxn'
        end if
*
        read *, iseed0
*   iseed = iseed0
*   = seed for random number generator
        read (12,*) nevent
*   = number of simulated events
        read (12,*) prob_nMin, dprob_n, nprob_n
*   = probability that a given site is a neutron

        END
*-----
SUBROUTINE init(n, nevent, prob_n, iprob_n,
&                peqSt, dpeq, npeq, pneqSt, dpneq, npneq)

        implicit double precision (A-H,O-Z)

        character lengthinfo*1, linfo*1, ninfo*3, probninfo*4,
&                numinfo*2, information*40, pneqStinfo*4

        read (12,'(a)') blank1
        read (12,'(a)') blank2
        read (12,'(8a,f8.0)') prob_n_info, prob_n_num
*
        read (12,*) peqSt, dpeq, npeq
        read (12,*) pneqSt, dpneq, npneq
*
        open(unit=13,file='runnumber.dat',form='formatted',status='old')
        read(13,'(a)') lengthinfo
        read(13,'(i2.2)') icurrentnumber
        close(13)

```

```

iprobn = probn * 1000
ipneqSt= pneqSt * 1000
write(ninfo,'(i3.3)') n
write(probninfo,'(i4.4)') iprobn
write(pneqStinfo,'(i4.4)') ipneqSt
write(numinfo,'(i2.2)') icurrentnumber
write(linfo,'(a)') lengthinfo

open(unit=14,file='zlog_'//ninfo//'_//probninfo//'_
& //pneqStinfo//'_//linfo//''//numinfo//'.dat',
& form='formatted',status='unknown')
open(unit=16,file='zpinf_'//ninfo//'_//probninfo//'_
& //pneqStinfo//'_//linfo//''//numinfo//'.dat',
& form='formatted',status='unknown')
open(unit=17,file='zpperc_'//ninfo//'_//probninfo//'_
& //pneqStinfo//'_//linfo//''//numinfo//'.dat',
& form='formatted',status='unknown')
open(unit=18,file='zffunc_'//ninfo//'_//probninfo//'_
& //pneqStinfo//'_//linfo//''//numinfo//'.dat',
& form='formatted',status='unknown')

if ((nevent-1) .eq. 0) then
  write (14,*)'#WARNING:standard deviation of average gives
& division by 0'
  write (16,*)'#WARNING:standard deviation of average gives
& division by 0'
  write (17,*)'#WARNING:standard deviation of average gives
& division by 0'
  write (18,*)'#WARNING:standard deviation of average gives
& division by 0'
endif

information = '** calc. with perc_prob00 on **'
write (14,*) information
write (14,'(a20,i5.4)') 'n          =' ,n
write (14,'(a20,e15.8)') 'probn_n  =' ,probn
write (14,'(a20,e15.8)') 'peqStart =' ,peqSt
write (14,'(a20,e15.8)') 'dpeq     =' ,dpeq
write (14,'(a20,i5.4)') 'npeq     =' ,npeq
write (14,'(a20,e15.8)') 'pneqStart =' ,pneqSt
write (14,'(a20,e15.8)') 'dpneq    =' ,dpneq
write (14,'(a20,i5.4)') 'npneq    =' ,npneq
write (14,*)
write (14,*)
END

```

```

-----
SUBROUTINE Perc(n, nevent, probn, peq, pneq)

```

```

implicit double precision (A-H,O-Z)

```

```

parameter (maxn = 128)
parameter (maxn1 = 129)
parameter (maxn2 = 16384)
parameter (maxn3 = 2097152)

```

```

logical neutron(maxn,maxn,maxn), maxperc
integer clusterNumber(0:maxn1,0:maxn1,0:maxn1)
double precision nn, np

```

```

do irun = 1,nevent
  call rndinit(iseed)
  call lattice(n, probn, iseed, neutron, nn, np)
  call rndinit(iseed)
  call PercChk(n, probn, peq, pneq, irun, iseed, neutron,
& ppbonds, pnbonds, maxClusSize, multip, maxperc)
& call StatIs(n, nevent, probn, peq, pneq, irun, nn, np,
& ppbonds, pnbonds, maxClusSize, multip, maxperc)

```

end do

END

SUBROUTINE rndinit(iseed)

implicit double precision (A-H,O-Z)

integer iseed, iseed0, iseed1

iseed0 = 0

iseed = 0

call system_clock(iseed0,iclock2,iclock3)

iseed = - (iseed0)

iseed1 = iseed

zinitret = ran1(iseed1)

write(14,'(a20,i13.12)')'randomseed =',iseed

write(14,*)

write(14,*)

END

SUBROUTINE lattice(n, prob_n, iseed1, neutron,
& theneutrons, theprotons)

implicit double precision (A-H,O-Z)

parameter (maxn = 128)

logical neutron(maxn,maxn,maxn), trueFalse

* Determine which sites are neutrons:

theneutrons = 0.D0

theprotons = 0.D0

do iz = 1,n

do iy = 1,n

do ix = 1,n

trueFalse = .TRUE.

if (ran1(iseed1) .lt. prob_n) then

theneutrons = theneutrons + 1.D0

else

trueFalse = .FALSE.

theprotons = theprotons + 1.D0

end if

neutron(ix,iy,iz) = trueFalse

end do

end do

end do

write(14,'(a20,e15.8)')'theneutrons =',theneutrons

write(14,'(a20,e15.8)')'theprotons =',theprotons

END

SUBROUTINE PercChk(n, prob_n, peq, pneq, irun, iseed,
& neutron, ppbonds, pnbonds, maxClusSize, multip, maxbotIn)

implicit double precision (A-H,O-Z)

parameter (maxn = 128)

parameter (maxn1 = 129)

parameter (maxn2 = 16384)

parameter (maxn3 = 2097152)

logical connected(maxn,maxn,maxn,3),

& neutron(maxn,maxn,maxn),

```

k      trueFalse, maxbotIn, maxtopIn

integer newPoint(maxn3,3),
k      clusterNumber(0:maxn1,0:maxn1,0:maxn1)
integer iseed, iseed1, hcln

*      Set random seed back to the initial value (cf Staufferbook p 73)
iseed1 = iseed
zinitret = ran1(iseed1)

*

n2 = n**2
n3 = n**3
hcln = (n3 + 1)
*      One more than highest possible clusterNumber if the whole lattice
*      is fragmented

*      Determine existing bonds
*      a: x-bonds -----
ppbonds = 0.DO
pnbonds = 0.DO
do iz = 1,n
  do iy = 1,n
    do ix = 1,n-1
      trueFalse = .FALSE.
      if (neutron(ix,iy,iz) .eqv. neutron(ix+1,iy,iz)) then
        if (ran1(iseed1) .lt. peq) then
          trueFalse = .TRUE.
          ppbonds = ppbonds + 1.DO
        end if
      else
        if (ran1(iseed1) .lt. pneq) then
          trueFalse = .TRUE.
          pnbonds = pnbonds + 1.DO
        end if
      end if
      connected(ix,iy,iz,1) = trueFalse
    end do
  end do
end do
*      b: y-bonds -----
do iz = 1,n
  do iy = 1,n-1
    do ix = 1,n
      trueFalse = .FALSE.
      if (neutron(ix,iy,iz) .eqv. neutron(ix,iy+1,iz)) then
        if (ran1(iseed1) .lt. peq) then
          trueFalse = .TRUE.
          ppbonds = ppbonds + 1.DO
        end if
      else
        if (ran1(iseed1) .lt. pneq) then
          trueFalse = .TRUE.
          pnbonds = pnbonds + 1.DO
        end if
      end if
      connected(ix,iy,iz,2) = trueFalse
    end do
  end do
end do
*      c: z-bonds -----
do iz = 1,n-1
  do iy = 1,n
    do ix = 1,n
      trueFalse = .FALSE.
      if (neutron(ix,iy,iz) .eqv. neutron(ix,iy,iz+1)) then
        if (ran1(iseed1) .lt. peq) then
          trueFalse = .TRUE.
          ppbonds = ppbonds + 1.DO
        end if
      end if
    end do
  end do
end do

```

```

        end if
      else
        if (ran1(iseed1) .lt. pneg) then
          trueFalse = .TRUE.
          pnbonds = pnbonds + 1.D0
        end if
      end if
      connected(ix,iy,iz,3) = trueFalse
    end do
  end do
end do
* Initialize connected values on boundaries as false
* a: x-bonds -----
do iz = 1,n
  do iy = 1,n
    connected(n,iy,iz,1) = .FALSE.
  enddo
enddo
* b: y-bonds -----
do iz = 1,n
  do ix = 1,n
    connected(ix,n,iz,2) = .FALSE.
  enddo
enddo
* c: z-bonds -----
do iy = 1,n
  do ix = 1,n
    connected(ix,iy,n,3) = .FALSE.
  enddo
enddo
*
* Assign the highest possible clusterNumber (hcln) to the surface
* lattice points, so that they are treated as already belonging to a
* cluster and are not dealt with in the cluster find algorithm
*
do iy = 0,n+1
  do ix = 0,n+1
    clusterNumber(ix,iy,0) = hcln
  end do
end do
do iy = 0,n+1
  do ix = 0,n+1
    clusterNumber(ix,iy,n+1) = hcln
  end do
end do
*
do iz = 0,n+1
  do ix = 0,n+1
    clusterNumber(ix,0,iz) = hcln
  end do
end do
do iz = 0,n+1
  do ix = 0,n+1
    clusterNumber(ix,n+1,iz) = hcln
  end do
end do
*
do iz = 0,n+1
  do iy = 0,n+1
    clusterNumber(0,iy,iz) = hcln
  end do
end do
do iz = 0,n+1
  do iy = 0,n+1
    clusterNumber(n+1,iy,iz) = hcln
  end do
end do
*

```



```

*   Assign the clusterNumber 0 (not part of any cluster) to all points
*   in the lattice that don't belong to the surface
*
do iz = 1,n
  do iy = 1,n
    do ix = 1,n
      clusterNumber(ix,iy,iz) = 0
    end do
  end do
end do
*   CLUSTER FIND SUBROUTINE-----
multip      = 0
maxClusSize = 0

do iz= 1,n
  do iy = 1,n
    do ix = 1,n
      IF(clusterNumber(ix,iy,iz) .eq. 0) then
*
****-new cluster, start -----
*
        clusterNumber(ix,iy,iz) = multip + 1
        newPoint(1,1) = ix
        newPoint(1,2) = iy
        newPoint(1,3) = iz
        IMINO = 1
        IMAXO = 1
*
1400      continue
        IMIN = IMAXO + 1
        IMAX = IMIN
        do I = IMINO,IMAXO
          IIX = newPoint(I,1)
          IYY = newPoint(I,2)
          IIZ = newPoint(I,3)

          IF(clusterNumber(IIX-1,IYY,IIZ) .eq. 0) THEN
            IF( connected(IIX-1,IYY,IIZ,1)) THEN
              newPoint(IMAX,1) = IIX-1
              newPoint(IMAX,2) = IYY
              newPoint(IMAX,3) = IIZ
              IMAX = IMAX + 1
              clusterNumber(IIX-1,IYY,IIZ) = multip+1
            END IF
          END IF
          IF(clusterNumber(IIX+1,IYY,IIZ) .eq. 0) THEN
            IF( connected(IIX,IYY,IIZ,1)) THEN
              newPoint(IMAX,1) = IIX+1
              newPoint(IMAX,2) = IYY
              newPoint(IMAX,3) = IIZ
              IMAX = IMAX + 1
              clusterNumber(IIX+1,IYY,IIZ) = multip+1
            END IF
          END IF
          IF(clusterNumber(IIX,IYY-1,IIZ) .eq. 0) THEN
            IF( connected(IIX,IYY-1,IIZ,2)) THEN
              newPoint(IMAX,1) = IIX
              newPoint(IMAX,2) = IYY-1
              newPoint(IMAX,3) = IIZ
              IMAX = IMAX + 1
              clusterNumber(IIX,IYY-1,IIZ) = multip+1
            END IF
          END IF
          IF(clusterNumber(IIX,IYY+1,IIZ) .eq. 0) THEN
            IF( connected(IIX,IYY,IIZ,2)) THEN
              newPoint(IMAX,1) = IIX
              newPoint(IMAX,2) = IYY+1
              newPoint(IMAX,3) = IIZ
            END IF
          END IF
        end do
      end do
    end do
  end do
end do

```

```

        IMAX          = IMAX + 1
        clusterNumber(IIX,IY+1,IIZ) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY,IIZ-1) .eq. 0) THEN
    IF( connected(IIX,IY,IIZ-1,3)) THEN
        newPoint(IMAX,1)   = IIX
        newPoint(IMAX,2)   = IY
        newPoint(IMAX,3)   = IIZ-1
        IMAX              = IMAX + 1
        clusterNumber(IIX,IY,IIZ-1) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY,IIZ+1) .eq. 0) THEN
    IF( connected(IIX,IY,IIZ,3)) THEN
        newPoint(IMAX,1)   = IIX
        newPoint(IMAX,2)   = IY
        newPoint(IMAX,3)   = IIZ+1
        IMAX              = IMAX + 1
        clusterNumber(IIX,IY,IIZ+1) = multip+1
    END IF
END IF

end do

IF(IMAX .NE. IMIN) THEN
    IMINO = IMIN
    IMAXO = IMAX - 1
    GOTO 1400
ENDIF
*   ; increase multiplicity
    multip = multip + 1
*   ; IMAXO contains cluster size
    if (imaxo .gt. maxClusSize) then
        maxClusSize = imaxo
        indexMax = multip
    end if
*
    END IF
end do
end do
END CLUSTER FIND SUBROUTINE
*   Check on Percolation of infinite cluster
maxtopIn = .FALSE.
maxbotIn = .FALSE.
do iy = 1,n
    do ix = 1,n
        if (clusterNumber(ix,iy,n) .eq. indexMax)
&            maxtopIn = .TRUE.
        end do
    end do
    if (maxtopIn) then
        do iy = 1,n
            do ix = 1,n
                if (clusterNumber(ix,iy,1) .eq. indexMax)
&                    maxbotIn = .TRUE.
                end do
            end do
        end if
    *
    pinf = dble(maxClusSize) / (dble(n)**3)
    write (14,'(a20,i5.4)') 'irun      =',irun
    write (14,'(a20,e15.8)') 'peq      =',peq
    write (14,'(a20,e15.8)') 'pneq     =',pneq
    write (14,'(a20,e15.8)') 'ppbonds  =',ppbonds
    write (14,'(a20,e15.8)') 'pnbonds  =',pnbonds
    write (14,'(a20,i13.12)') 'maxClSize=',maxClusSize

```

```

write (14,'(a20,e15.8)') 'pinf      =',pinf
write (14,'(a20,i13.12)')'multip   =',multip
write (14,'(a20,12)')    'maxbotIn =',maxbotIn
write (14,*)
write (14,*)

```

END

```

-----
SUBROUTINE Statis(n, nevent, prob_n, peq, pneq, irun, nn, np,
& ppbonds, pnbonds, maxClusSize, multip, maxperc)

```

```

implicit double precision (A-H,O-Z)

```

```

parameter (maxn = 128)
parameter (maxn1 = 129)
parameter (maxn2 = 16384)
parameter (maxn3 = 2097152)

```

```

logical maxperc
double precision nn, np, anu, invanu

```

```

SAVE sumP, sumN, sumPPBonds, sumPNBonds, sumInfClus, sm2InfClus,
& sumPercP, sm2PercP, sumMult, sm2Mult

```

```

if (irun .eq. 1) then
  sumP = 0.D0
  sumN = 0.D0
  aveP = 0.D0
  aveN = 0.D0
  sumPPBonds = 0.D0
  sumPNBonds = 0.D0
  sumInfClus = 0.D0
  sm2InfClus = 0.D0
  aveInfClus = 0.D0
  av2InfClus = 0.D0
  stdInfClus = 0.D0
  sumPercP = 0.D0
  sm2PercP = 0.D0
  avePercP = 0.D0
  av2PercP = 0.D0
  stdPercP = 0.D0
  sumMult = 0.D0
  sm2Mult = 0.D0
  aveMult = 0.D0
  av2Mult = 0.D0
  stdMult = 0.D0
endif

```

*

* Summation

*

* Particles

```

sumP = sumP + np
sumN = sumN + nn

```

*

Bonds

```

sumPPBonds = sumPPBonds + ppbonds
sumPNBonds = sumPNBonds + pnbonds

```

*

Percolation

```

if (maxperc) sumInfClus = sumInfClus + dble(maxClusSize)
if (maxperc) sm2InfClus = sm2InfClus + (dble(maxClusSize))**2
if (maxperc) sumPercP = sumPercP + 1.D0
if (maxperc) sm2PercP = sm2PercP + 1.D0
sumMult = sumMult + dble(multip)
sm2Mult = sm2Mult + (dble(multip))**2

```

*

* Averaging

*

```

if (irun .eq. nevent) then

```

```

        if ((nevent-1) .eq. 0) then
            srt = 0.1D-20
        else
            srt = sqrt(dble(nevent-1))
        endif
*   Particles
        aveP = sumP / dble(nevent)
        aveN = sumN / dble(nevent)
*   Bonds
        avePPBonds = sumPPBonds / dble(nevent)
        avePNBonds = sumPNBonds / dble(nevent)
*   Percolation
        aveInfClus = (sumInfClus / (dble(n)**3)) / dble(nevent)
        av2InfClus = sm2InfClus / ((dble(n)**3)**2)
        stdInfClus = sqrt(abs(av2InfClus/dble(nevent)-aveInfClus**2))
    & /srt
        avePercP = sumPercP / dble(nevent)
        av2PercP = sm2PercP
        stdPercP = sqrt(abs(av2PercP / dble(nevent) - avePercP**2))
    & /srt
        aveMult = sumMult / (dble(n)**3) / dble(nevent)
        av2Mult = sm2Mult / ((dble(n)**3)**2)
        stdMult = sqrt(abs(av2Mult / dble(nevent) - aveMult**2))
    & / srt
*
        anu = 2.D0*prob_n*(1.D0-prob_n)
        invanu = (1.D0 - anu)
        pplus = invanu*peq + anu*pneq
*
*   Output
*   LogFile
        write(14,'(a20,e15.8)')'anu =',anu
        write(14,'(a20,e15.8)')'invanu=',invanu
        write(14,'(a20,e15.8)')'pplus =',pplus
        write(14,'(a20,2e15.8)')'pinf, stdpinf =',aveInfClus, stdInfClus
        write(14,'(a20,2e15.8)')'pperc, stdpperc=',avePercP, stdPercP
        write(14,'(a20,2e15.8)')'ffunc, stdffunc=',aveMult, stdMult
*   Files
        write (16,'(5e15.8)') peq, pneq, pplus,
    & aveInfClus, stdInfClus
        write (17,'(5e15.8)') peq, pneq, pplus,
    & avePercP, stdPercP
        write (18,'(5e15.8)') peq, pneq, pplus,
    & aveMult, stdMult
        endif
    END
-----

```

```

FUNCTION rani(idum)

```

```

    IMPLICIT DOUBLE PRECISION (A-H,O-Z)

```

```

    INTEGER idum, IA, IM, IQ, IR, NTAB, NDIV

```

```

    DOUBLE PRECISION rani, AM, EPS, RNMX

```

```

    PARAMETER (IA=16807, IM=2147483647, AM=1./IM, IQ=127773, IR=2836,

```

```

    & NTAB=32, NDIV=1+(IM-1)/NTAB, EPS=1.2d-7, RNMX=1.d0-EPS)

```

```

    INTEGER j, k, iv(NTAB), iy

```

```

    SAVE iv, iy

```

```

    DATA iv /NTAB*0/, iy /0/

```

```

    if (idum .le. 0 .or. iy .eq. 0) then

```

```

        idum=max(-idum,1)

```

```

        do j=NTAB+8, 1, -1

```

```

            k=idum/IQ

```

```

            idum=IA*(idum-k*IQ)-IR*k

```

```

            if (idum .lt. 0) idum=idum+IM

```

```

            if (j .le. NTAB) iv(j)=idum

```

```

        enddo

```

```

        iy=iv(1)

```

```

endif
k=idum/IQ
idum=IA*(idum-k+IQ)-IR*k
if (idum .lt. 0) idum=idum+IM
j=1+iy/NDIV
iy=iv(j)
iv(j)=idum
rani=min(AM*iy,RNMX)
return

END

```

A.2 perc_ppintv0477.f

The second program, `perc_ppintv0477.f` was written to accommodate the more specific need of determining the critical value of the bond density, p_+^c , through determination of p_-^c . Similar versions aiming at the critical value of p_{\neq} and f_b respectively have also been used. Again, for a more thorough discussion of the programs features, we refer to Sec. 3.3.

```

program perc_ppintv0477

*   uses fortran 77 conventions
*   varies prob_n, pp at fixed pn and determines ppc, pplus
*   uses a random number generator taken from numerical recipes in
*   fortran 2nd ed.: rani(iseed), modified to use double precision
*   Lattice population with neutrons has own subroutine: lattice

implicit double precision (A-H,O-Z)

call readpar(n, nevent, prob_nMin, dprob_n, nprob_n, delta,
&           zlambda)
*-----
*   Loop over prob_n:
*-----
  prob_n = prob_nMin
  do iprob_n = 0, nprob_n
    call init(n, nevent, prob_n, iprob_n, delta, zlambda, apeqSt,
&           bpeqSt, pneqSt, dpneq, npneq)
    pneq = pneqSt
    do ipneq = 0, npneq
      call iter(n, nevent, prob_n, apeqSt, bpeqSt, pneq,
&             delta, zlambda)
      pneq = pneq + dpneq
    end do
    prob_n = prob_n + dprob_n
  end do
*-----
*   End Loop over prob_n:
*-----
end

*-----
SUBROUTINE readpar(n, nevent, prob_nMin, dprob_n, nprob_n, delta,
&               zlambda)

implicit double precision (A-H,O-Z)

parameter (maxn = 128)

*   input parameters:
*
open(unit=12,file='parall.dat',status='old')

```

```

      read (12,*) n
*      = number of lattice sites in one direction
      if (n .gt. maxn) then
        print *, ' > Fatal Error: n must be less or equal maxn'
      end if
*      read *, iseed0
*      iseed = iseed0
*      = seed for random number generator
      read (12,*) nevent
*      = number of simulated events
      read (12,*) prob_nMin, dprob_n, nprob_n
*      = probability that a given site is a neutron
      read (12,*) delta
*      precision to be reached in the final interval step
      read (12,*) zlambda
*      interval division

      END
-----
      SUBROUTINE init(n, nevent, prob_n, iprob_n, delta, zlambda,
&      apeqSt, bpeqSt, pneqSt, dpneq, npneq)

      implicit double precision (A-H,O-Z)

      character lengthinfo*1, linfo*1, ninfo*3, probninfo*4,
&      numinfo*2, information*40, pneqStinfo*4

      read (12,'(a)') blank1
      read (12,'(a)') blank2
      read (12,'(8a,f8.0)') prob_n_info, prob_n_num
*
      read (12,*) apeqSt, bpeqSt
      read (12,*) pneqSt, dpneq, npneq
*
      open(unit=13,file='runnumber.dat',form='formatted',status='old')
      read(13,'(a)') lengthinfo
      read(13,'(i2.2)') icurrentnumber
      close(13)

      iprobn = prob_n * 1000
      ipneqSt= pneqSt * 1000
      write(ninfo,'(i3.3)') n
      write(probninfo,'(i4.4)') iprobn
      write(pneqStinfo,'(i4.4)') ipneqSt
      write(numinfo,'(i2.2)') icurrentnumber
      write(linfo,'(a)') lengthinfo

      open(unit=14,file='zlog_'//ninfo//'_//probninfo//'_
&      //pneqStinfo//'_//linfo//''//numinfo//'.dat',
&      form='formatted',status='unknown')
      open(unit=16,file='zpplusclog_'//ninfo//'_//probninfo//'_
&      //pneqStinfo//'_//linfo//''//numinfo//'.dat',
&      form='formatted',status='unknown')
      if (iprob_n .eq. 0) then
        open(unit=17,file='zpeqc_'//ninfo//'_//probninfo//'_
&      //pneqStinfo//'_//linfo//''//numinfo//'.dat',
&      form='formatted',status='unknown')
        open(unit=18,file='zpplusc_'//ninfo//'_//probninfo//'_
&      //pneqStinfo//'_//linfo//''//numinfo//'.dat',
&      form='formatted',status='unknown')
      endif

      if ((nevent-1) .eq. 0) then
        write (14,*)'#WARNING:standard deviation of average gives
& division by 0'
        write (16,*)'#WARNING:standard deviation of average gives
& division by 0'
        write (17,*)'#WARNING:standard deviation of average gives

```

```

& division by 0'
  write (18,*)'#WARNING:standard deviation of average gives
& division by 0'
endif

```

```

information = '** calc. with perc_ppintv0477 on **'
write (14,*) information
write (14,'(a20,i4.4)') 'n      =',n
write (14,'(a20,e15.8)')'delta  =',delta
write (14,'(a20,e15.8)')'zlambda =',zlambda
write (14,'(a20,e15.8)')'prob_n  =',prob_n
write (14,'(a20,e15.8)')'apeqStart=',apeqSt
write (14,'(a20,e15.8)')'bpeqStart=',bpeqSt
write (14,'(a20,e15.8)')'pneqStart=',pneqSt
write (14,'(a20,e15.8)')'dpneq   =',dpneq
write (14,'(a20,i4.4)') 'npneq   =',npneq
write (14,*)
write (14,*)
END

```

```

-----
SUBROUTINE iter(n, nevent, prob_n, apeqSt, bpeqSt, pneq,
& delta, zlambda)

```

```

implicit double precision (A-H,O-Z)

```

```

parameter (maxn = 128)
logical neutron(maxn,maxn,maxn)
integer perc, percount
double precision invanu

```

```

sumpeqc = 0.D0
sm2peqc = 0.D0
sumplusplus = 0.D0
sm2plusplus = 0.D0

```

```

anu = 2.D0*prob_n*(1.D0-prob_n)
invanu = (1.D0 - anu)

```

```

write (14,'(a20,e15.8)')'anu      =',anu

```

```

do irun = 1,nevent
  call rndinit(iseed)
  call lattice(n, prob_n, iseed, neutron)
  call rndinit(iseed)
  a = apeqSt
  b = bpeqSt
  percount = 0
  do while ((b - a) .gt. delta)
    c = zlambda*b + (1-zlambda)*a
    call PercChk(n, prob_n, c, pneq, irun, iseed, neutron, perc)
    if (perc .EQ. 1) then
      b = c
      percount = percount + 1
    else
      a = c
    endif
  end do
  peqc = c
  write(14,'(a20,e15.8)')'anu',anu
  write(14,'(a20,e15.8)')'invanu',invanu
  write(14,'(a20,e15.8)')'peqc',peqc
  pplusplus = invanu*peqc + anu*pneq
  write(14,'(a20,e15.8)')'plusplus',plusplus
  write (16,'(i4.4,3e15.8)') irun,pneq,peqc,plusplus
  sumpeqc = sumpeqc + peqc
  sm2peqc = sm2peqc + (peqc)**2
  sumplusplus = sumplusplus + pplusplus

```

```

    sm2plusplus = sm2plusplus + (plusplus)**2
end do
*
srt = sqrt(dble(nevent-1))
if ((nevent-1) .eq. 0) then
    srt = 0.1D-20
endif
avpeqc = sumpeqc / dble(nevent)
stdpeqc= sqrt(abs(sm2peqc/dble(nevent)-avpeqc**2))/srt
avplusplus = sumplusplus / dble(nevent)
stdplusplus= sqrt(abs(sm2plusplus/dble(nevent)-avplusplus**2))/srt
deltaplus = invanu*delta
*
write (17,'(i4.4,5e15.8)') n,prob_n, pneq, avpeqc, delta, stdpeqc
write (18,'(i4.4,5e15.8)') n,prob_n, pneq, avplusplus, deltaplus,
&    stdplusplus
END
*-----

```

```

SUBROUTINE rndinit(iseed)

implicit double precision (A-H,O-Z)

integer iseed, iseed0, iseed1

iseed0 = 0
iseed = 0
call system_clock(iseed0,iclock2,iclock3)
iseed = - (iseed0)
iseed1 = iseed
zinitret = ran1(iseed1)
write(14,'(a20,i13.12)')'randomseed =',iseed

write(14,*)
write(14,*)

END
*-----

```

```

SUBROUTINE lattice(n, prob_n, iseed1, neutron)

implicit double precision (A-H,O-Z)

parameter (maxn = 128)
logical neutron(maxn,maxn,maxn), trueFalse
*
Determine which sites are neutrons:
theneutrons = 0.DO
theprotons = 0.DO
sumNeutron = 0.DO
sumProton = 0.DO

do iz = 1,n
do iy = 1,n
do ix = 1,n
    trueFalse = .TRUE.
    if (ran1(iseed1) .lt. prob_n) then
        theneutrons = theneutrons + 1.DO
    else
        trueFalse = .FALSE.
        theprotons = theprotons + 1.DO
    end if
    neutron(ix,iy,iz) = trueFalse
end do
end do
sumNeutron = sumNeutron + theneutrons

```



```

sumProton = sumProton + theprotons
write(14,'(a20,e15.8)')sumNeutron = ',sumNeutron
write(14,'(a20,e15.8)')sumProton = ',sumProton
END

```

```

-----
SUBROUTINE PercChk(n, prob_n, peq, pneq, irun, iseed,
& neutron, perc)

implicit double precision (A-H,O-Z)

parameter (maxn = 128)
parameter (maxn1 = 129)
parameter (maxn2 = 16384)
parameter (maxn3 = 2097152)

logical connected(maxn,maxn,maxn,3),
& neutron(maxn,maxn,maxn),
& trueFalse

integer newPoint(maxn3,3),
& clusterNumber(0:maxn1,0:maxn1,0:maxn1)
integer iseed, perc, hcln

* Set random seed back to the initial value (cf Staufferbook p 73)
iseed1 = iseed
zinitret = ran1(iseed1)
*

n2 = n**2
n3 = n**3
hcln = (n3 + 1)
* One more than highest possible clusterNumber if the whole lattice
* is fragmented

* Determine existing bonds
* a: x-bonds -----
ppbonds = 0.DO
pnbonds = 0.DO
do iz = 1,n
do iy = 1,n
do ix = 1,n-1
trueFalse = .FALSE.
if (neutron(ix,iy,iz) .eqv. neutron(ix+1,iy,iz)) then
if (ran1(iseed1) .lt. peq) then
trueFalse = .TRUE.
ppbonds = ppbonds + 1.DO
end if
else
if (ran1(iseed1) .lt. pneq) then
trueFalse = .TRUE.
pnbonds = pnbonds + 1.DO
end if
end if
connected(ix,iy,iz,1) = trueFalse
end do
end do
end do
* b: y-bonds -----
do iz = 1,n
do iy = 1,n-1
do ix = 1,n
trueFalse = .FALSE.
if (neutron(ix,iy,iz) .eqv. neutron(ix,iy+1,iz)) then
if (ran1(iseed1) .lt. peq) then
trueFalse = .TRUE.
ppbonds = ppbonds + 1.DO
end if
else

```

```

        if (ran1(iseed1) .lt. pneq) then
            trueFalse = .TRUE.
            pnbonnds = pnbonnds + 1.D0
        end if
    end if
    connected(ix,iy,iz,2) = trueFalse
end do
end do
end do
* c: z-bonds -----
do iz = 1,n-1
    do iy = 1,n
        do ix = 1,n
            trueFalse = .FALSE.
            if (neutron(ix,iy,iz) .eqv. neutron(ix,iy,iz+1)) then
                if (ran1(iseed1) .lt. peq) then
                    trueFalse = .TRUE.
                    ppbonnds = ppbonnds + 1.D0
                end if
            else
                if (ran1(iseed1) .lt. pneq) then
                    trueFalse = .TRUE.
                    pnbonnds = pnbonnds + 1.D0
                end if
            end if
            connected(ix,iy,iz,3) = trueFalse
        end do
    end do
end do
* Initialize connected values on boundaries as false
* a: x-bonds -----
do iz = 1,n
    do iy = 1,n
        connected(n,iy,iz,1) = .FALSE.
    enddo
enddo
* b: y-bonds -----
do iz = 1,n
    do ix = 1,n
        connected(ix,n,iz,2) = .FALSE.
    enddo
enddo
* c: z-bonds -----
do iy = 1,n
    do ix = 1,n
        connected(ix,iy,n,3) = .FALSE.
    enddo
enddo
*
* Assign the highest possible clusterNumber (hcln) to the surface lattice
* points, so that they are treated as already belonging to a
* cluster and are not dealt with in the cluster find algorithm
*
do iy = 0,n+1
    do ix = 0,n+1
        clusterNumber(ix,iy,0) = hcln
    end do
end do
do iy = 0,n+1
    do ix = 0,n+1
        clusterNumber(ix,iy,n+1) = hcln
    end do
end do
*
do iz = 0,n+1
    do ix = 0,n+1
        clusterNumber(ix,0,iz) = hcln
    end do
end do

```

```

end do
do iz = 0,n+1
  do ix = 0,n+1
    clusterNumber(ix,n+1,iz) = hcln
  end do
end do
*
do iz = 0,n+1
  do iy = 0,n+1
    clusterNumber(0,iy,iz) = hcln
  end do
end do
do iz = 0,n+1
  do iy = 0,n+1
    clusterNumber(n+1,iy,iz) = hcln
  end do
end do
*
* Assign the clusterNumber 0 (not part of any cluster) to all points in
* the lattice that don't belong to the surface
*
do iz = 1,n
  do iy = 1,n
    do ix = 1,n
      clusterNumber(ix,iy,iz) = 0
    end do
  end do
end do
* CLUSTER FIND SUBROUTINE-----
perc      = 0
multip    = 0
ipclsize  = 0
maxClusSize = 0

iz=1
do iy = 1,n
  do ix = 1,n
    IF(clusterNumber(ix,iy,iz) .eq. 0) then
*
****-new cluster, start -----
*
      clusterNumber(ix,iy,iz) = multip + 1
      newPoint(1,1) = ix
      newPoint(1,2) = iy
      newPoint(1,3) = iz
      IMINO = 1
      IMAXO = 1
*
1400      continue
      IMIN = IMAXO + 1
      IMAX = IMIN
      do I = IMINO, IMAXO
        IIX = newPoint(I,1)
        IIY = newPoint(I,2)
        IIZ = newPoint(I,3)

        IF(clusterNumber(IIX-1,IIY,IIZ) .eq. 0) THEN
          IF( connected(IIX-1,IIY,IIZ,1)) THEN
            newPoint(IMAX,1) = IIX-1
            newPoint(IMAX,2) = IIY
            newPoint(IMAX,3) = IIZ
            IMAX = IMAX + 1
            clusterNumber(IIX-1,IIY,IIZ) = multip+1
          END IF
        END IF
        IF(clusterNumber(IIX+1,IIY,IIZ) .eq. 0) THEN
          IF( connected(IIX,IIY,IIZ,1)) THEN
            newPoint(IMAX,1) = IIX+1

```

```

        newPoint(IMAX,2)      = IY
        newPoint(IMAX,3)      = IZ
        IMAX                   = IMAX + 1
        clusterNumber(IIX+1,IY,IZ) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY-1,IZ) .eq. 0) THEN
    IF( connected(IIX,IY-1,IZ,2) ) THEN
        newPoint(IMAX,1)      = IIX
        newPoint(IMAX,2)      = IY-1
        newPoint(IMAX,3)      = IZ
        IMAX                   = IMAX + 1
        clusterNumber(IIX,IY-1,IZ) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY+1,IZ) .eq. 0) THEN
    IF( connected(IIX,IY,IZ,2) ) THEN
        newPoint(IMAX,1)      = IIX
        newPoint(IMAX,2)      = IY+1
        newPoint(IMAX,3)      = IZ
        IMAX                   = IMAX + 1
        clusterNumber(IIX,IY+1,IZ) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY,IZ-1) .eq. 0) THEN
    IF( connected(IIX,IY,IZ-1,3) ) THEN
        newPoint(IMAX,1)      = IIX
        newPoint(IMAX,2)      = IY
        newPoint(IMAX,3)      = IZ-1
        IMAX                   = IMAX + 1
        clusterNumber(IIX,IY,IZ-1) = multip+1
    END IF
END IF
IF(clusterNumber(IIX,IY,IZ+1) .eq. 0) THEN
    IF( connected(IIX,IY,IZ,3) ) THEN
        newPoint(IMAX,1)      = IIX
        newPoint(IMAX,2)      = IY
        newPoint(IMAX,3)      = IZ+1
        IMAX                   = IMAX + 1
        clusterNumber(IIX,IY,IZ+1) = multip+1
        IF(IIZ+1 .EQ. n) THEN
            perc      = 1
            multip    = multip+1
            ipclsize  = imaxo
            write (14,'(a20,i5.4)') 'irun      =',irun
            write (14,'(a20,e15.8)') 'peq      =',peq
            write (14,'(a20,e15.8)') 'pneq     =',pneq
            write (14,'(a20,e15.8)') 'ppbonds  =',ppbonds
            write (14,'(a20,e15.8)') 'pnbonds  =',pnbonds
            write (14,'(a20,i13.12)') 'multip   =',multip
            write (14,'(a20,i13.12)') 'ipclsize =',
                &
                ipclsize
            write (14,'(a20,i2.1)') 'perc      =',perc
            write (14,*)
            write (14,*)
            RETURN
        END IF
    END IF
END IF
end do

IF(IMAX .NE. IMIN) THEN
    IMINO = IMIN
    IMAXO = IMAX - 1
    GOTO 1400
ENDIF
* ; increase multiplicity

```

```

multip = multip + 1
* ; IMAX0 contains cluster size
      if (imaxo .gt. maxClusSize) then
          maxClusSize = imaxo
          indexMax = multip
      end if
*
      END IF
    end do
  end do
* END CLUSTER FIND SUBROUTINE
  write (14,'(a20,i5.4)') 'irun      =',irun
  write (14,'(a20,e15.8)') 'peq      =',peq
  write (14,'(a20,e15.8)') 'pneq     =',pneq
  write (14,'(a20,e15.8)') 'ppbonds  =',ppbonds
  write (14,'(a20,e15.8)') 'pnbonds  =',pnbonds
  write (14,'(a20,i13.12)') 'multip   =',multip
  write (14,'(a20,i13.12)') 'ipclsize =',ipclsize
  write (14,'(a20,i2.1)')  'perc     =',perc
  write (14,*)
  write (14,*)

```

END

FUNCTION rani(idum)

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

INTEGER idum, IA, IM, IQ, IR, NTAB, NDIV

DOUBLE PRECISION rani, AM, EPS, RNMX

PARAMETER (IA=16807, IM=2147483647, AM=1./IM, IQ=127773, IR=2836,

& NTAB=32, NDIV=1+(IM-1)/NTAB, EPS=1.2d-7, RNMX=1.d0-EPS)

INTEGER j, k, iv(NTAB), iy

SAVE iv, iy

DATA iv /NTAB*0/, iy /0/

if (idum .le. 0 .or. iy .eq. 0) then

idum=max(-idum,1)

do j=NTAB+8, 1, -1

k=idum/IQ

idum=IA*(idum-k*IQ)-IR*k

if (idum .lt. 0) idum=idum+IM

if (j .le. NTAB) iv(j)=idum

enddo

iy=iv(1)

endif

k=idum/IQ

idum=IA*(idum-k*IQ)-IR*k

if (idum .lt. 0) idum=idum+IM

j=1+iy/NDIV

iy=iv(j)

iv(j)=idum

rani=min(AM*iy,RNMX)

return

END

Bibliography

- [ARRS79] P. Agrawal, S. Redner, P. J. Reynolds, and H. E. Stanley, *J. Phys. C* **12** (1979).
- [Bab97] F. Babalievski, cond-mat/9711304 (1997).
- [Bau] W. Bauer, (private communication).
- [Bau88] W. Bauer, *Phys. Rev. C* **38** (1988), 1297.
- [Baued] W. Bauer, Proceedings of the Workshop on Nuclear Matter in Different Phases and Transitions, (Les Houches, France), 1999, to be published.
- [BB95] W. Bauer and A. Botvina, *Phys. Rev. C* **52** (1995), R1760.
- [BBDG87] W. Bauer, G. F. Bertsch, and S. Das Gupta, *Phys. Rev. Lett.* **58** (1987), 863.
- [BC89] P. Bak and K. Chen, *Physica D* **38** (1989), 5.
- [BDMP85] W. Bauer, D. R. Dean, U. Mosel, and U. Post, *Phys. Lett.* **150 B** (1985), 53.
- [BF94] W. Bauer and W. A. Friedman, ??/nucl-th/9411012 ?? (1994), ??
- [BF95] W. Bauer and W. A. Friedman, *Phys. Rev. Lett.* **75** (1995), 767.
- [BH57] S. R. Broadbent and J. M. Hammersley, *Percolation processes i. crystals and mazes.*, Proceedings of the Cambridge Philosophical Society, vol. 53, 1957, pp. 629–641.
- [BH97] K. Binder and D. W. Heermann (eds.), *Monte carlo simulation in statistical physics, an introduction*, 3 rd ed., Springer Verlag, Berlin, 1997.
- [Bin79] K. Binder (ed.), *Monte carlo methods in statistical physics*, Springer Verlag, Heidelberg, 1979.
- [BPDM86] W. Bauer, U. Post, D. R. Dean, and U. Mosel, *Nucl. Phys. A* **452** (1986), 699.
- [CB97] R. Cont and J. P. Bouchaud, cond-mat/9712318 (1997).
- [CC99] J. Cardy and F. Colaiori, *Phys. Rev. Lett.* **82** (1999), 2232.

- [CSK79] A. Coniglio, H. E. Stanley, and W. Klein, *Phys. Rev. Lett.* **42** (1979), 518.
- [Deb97] J.-M. Debierre, *Phys. Rev. Lett.* **78** (1997), 3145.
- [DG72a] C. Domb and M. S. Green (eds.), *Phase transitions and critical phenomena*, vol. 2, Academic Press, 1972.
- [DG72b] C. Domb and M. S. Green (eds.), *Phase transitions and critical phenomena*, vol. 5a, Academic Press, 1972.
- [Dua90] J. A. M. S. Duarte, *Z. Phys.* **80** (1990), 299.
- [Dup99] B. Duplantier, cond-mat/9901008 (1999).
- [Dur88] R. Durrett, *Lecture notes on particle systems and percolation*, Wadsworth and Brooks/Cole, 1988.
- [DZA83] G. Deutscher, R. Zallen, and J. Adler (eds.), *Percolation structures and processes*, Adam Hilger, Bristol, 1983.
- [FE61] M. E. Fisher and J. W. Essam, *J. Math. Phys.* **2** (1961), 609–619.
- [Fed88] J. Feder, *Fractals*, Plenum Press, 1988.
- [Fis61] M. E. Fisher, *J. Math. Phys.* **2** (1961), 620–627.
- [Flo41] P. J. Flory, *J. Am. Chem. Soc.* **63** (1941), 3083.
- [Gar95] C. Garrod, *Statistical mechanics and thermodynamics*, Oxford University Press, 1995.
- [GBP98] T. Gharib, W. Bauer, and S. Pratt, *Phys. Lett. B* **444** (1998), 231.
- [GGH92] S. Das Gupta, C. Gale, and K. Haglin, nucl-th/9210020 (1992).
- [GM96] S. Galam and A. Mauger, *Phys. Rev. E* (1996).
- [GM97] S. Galam and A. Mauger, *Phys. Rev. E* **56** (1997), 322.
- [Gri70] R. B. Griffiths, *Phys. Rev. Lett.* **24** (1970), 1949.
- [Gri89] G. Grimmett, *Percolation*, Springer Verlag, New York, 1989.
- [Gri99] G. Grimmett, *Percolation*, 2nd ed., Springer Verlag, Berlin, 1999.
- [Ham57] J. M. Hammersley, *Percolation processes. lower bounds for the critical probability*, *Annals of the Mathematical Statistics*, vol. 28, 1957, pp. 790–795.
- [Ham59] J. M. Hammersley, *Bornes supérieures de la probabilité critique dans un processus de filtration*, *Le Calcul des Probabilité et ses Applications*, CNRS, Paris, 1959, pp. 17–37.
- [HB99] H. M. Harreis and W. Bauer, cond-mat/9907330 (1999).

- [HBM97] J. Hoshen, M. W. Berry, and K. S. Minser, *Phys. Rev. E* **56** (1997), 1455.
- [HH78] J. W. Halley and W. K. Holcomb, *Phys. Rev. Lett.* **40** (1978), 1670.
- [HK76] J. Hoshen and R. Kopelman, *Phys. Rev. B* **14** (1976), 3438.
- [HKM78] J. Hoshen, R. Kopelman, and E. M. Monberg, *J. Statist. Phys.* **19** (1978), 219.
- [HS81] D. W. Heermann and D. Stauffer, *Z. Phys.* **44** (1981), 339.
- [HSB⁺79] J. Hoshen, D. Stauffer, G. H. Bishop, R. J. Harrison, and G. P. Quinn, *J. Phys. A* **12** (1979).
- [Hua87] K. Huang, *Statistical mechanics*, 2nd ed., John Wiley and Sons, 1987.
- [Ios95] A. S. Ioselevich, *Phys. Rev. Lett.* **74** (1995), 1411.
- [KADS83] A. Kapiltunik, A. Aharony, G. Deutscher, and D. Stauffer, *J. Phys. A* **16** (1983), L269–L274.
- [KBK97] G. Kortemeyer, W. Bauer, and G. J. Kunde, *Phys. Rev. C* **55** (1997), 2730.
- [Kes82] H. Kesten, *Percolation theory for mathematicians*, Birkhäuser, 1982.
- [Kes87] H. Kesten (ed.), *Percolation theory and ergodic theory of infinite particle systems*, Springer-Verlag, 1987.
- [Kre91] U. Krengel, *Einführung in die Wahrscheinlichkeitstheorie und Statistik*, 3rd revised ed., Vieweg, 1991.
- [LZ98] C. D. Lorenz and R. M. Ziff, *Phys. Rev. E* **57** (1998), 230.
- [Nol93] W. Nolting, *Grundkurs Theoretische Physik, 4 Thermodynamik*, 2nd revised ed., Verlag Zimmermann-Neufang, 1993.
- [Nol98] W. Nolting, *Grundkurs Theoretische Physik, 6 Statistische Physik*, 3rd ed., Vieweg Verlag, 1998.
- [OCG⁺78] H. Ottavi, J. Clerc, G. Giraud, J. Roussenq, E. Guyon, and C. D. Mitescu, *J. Phys. C* **11** (1978), 1311.
- [Pat96] R. K. Pathria, *Statistical mechanics*, 2nd ed., Butterworth-Heinemann, 1996.
- [PTVF92] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical recipes in fortran*, 2nd ed., Cambridge University Press, 1992.
- [QBH76] G. P. Quinn, G. H. Bishop, and R. J. Harrison, *J. Phys. A* **9** (1976), L 9.
- [SA94] D. Stauffer and A. Aharony, *Introduction to percolation theory*, revised 2nd ed., Taylor and Francis, London, 1994.

- [Sah94] M. Sahimi, *Applications of percolation theory*, Taylor and Francis, London, 1994.
- [SE64] M. F. Sykes and J. W. Essam, *J. Math. Phys.* **5** (1964), 1117.
- [Sin81] YA. G. Sinai, *Theory of phase transitions: Rigorous results*, Pergamon Press, 1981.
- [Sta71] H. E. Stanley, *Introduction to phase transitions and critical phenomena*, Oxford University Press, 1971.
- [Sta79] D. Stauffer, *Phys. Rep.* **54** (1979), 3.
- [Sti89] K. Stierstadt, *Physik der Materie*, VCH Weinheim, 1989.
- [Sto43] W. H. Stockmayer, *J. Chem. Phys.* **11** (1943), 45.
- [vB99] J. von Bergmann, (private communication), 1999.
- [vdM97] S. C. van der Marck, *Phys. Rev. E* **55** (1997), 1514.
- [vdM98] S. C. van der Marck, *Intl. J. Mod. Phys. C* **9** (1998), 529.
- [WP78] H. J. Wintle and P. H. Puhach, *J. Statist. Phys.* **18** (1978), 557.
- [Yeo92] J. M. Yeomans, *Statistical mechanics of phase transitions*, Clarendon Press, Oxford, 1992.
- [Zal77] R. Zallen, *Phys. Rev. B* **16** (1977), 1426.
- [Zal83] R. Zallen, *The physics of amorphous solids*, John Wiley, New York, 1983.
- [Zif92] R. M. Ziff, *Phys. Rev. Lett.* **69** (1992), 2670.

MICHIGAN STATE UNIV. LIBRARIES



31293018209092