

Percolation on square lattice by a class of ballistic deposition and their universality classes



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I would like to dedicate this thesis to my loving parents . . .

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgments. All the codes to simulate the model and analyze the data are written by me. This dissertation contains about 36,000 words including appendices, bibliography, footnotes, tables and equations and has about 70 figures.

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Abstract

This thesis consists of two parts. First, we redefined the 60 years old site percolation focusing primarily on entropy which quantifies the degree of disorder and order parameter that measures the extent of order. Note that being two opposite quantities they can neither be minimum nor be maximum at the same time which is perfectly consistent with bond percolation. However, the same is not true for traditional site percolation as we find that entropy and order parameter are both zero at occupation probability $p = 0$ and the way entropy behaves it violates the second law of thermodynamics. To overcome this we redefine the site percolation where we occupy sites to connect bonds and we measure cluster size by the number of bonds connected by occupied sites. This resolves the problem without affecting any of the existing known results whatsoever.

Second, we investigate percolation by random sequential ballistic deposition (RSBD) on a square lattice with interaction range upto second nearest neighbors. In percolation by random sequential deposition process a site is picked at random and we occupy it if the site is empty else the trial attempt is rejected. In sequential ballistic deposition we modify the rejection criteron. That is, instead of rejecting the trial attempt we let roll over the occupied particle along one of the four directions at random which is then occupied if that site is empty else the attempt rejected. The critical points p_c and all the necessary critical exponents α , β , γ , ν etc. are obtained numerically for each range of interactions. Like in its thermal counterpart, we find that the critical exponents of RSBD depend on the range of interactions and for a given range of interaction they obey the Rushbrooke inequality. Besides, we obtain the fractal dimension d_f that characterizes the spanning cluster at p_c . Our results suggest that the RSBD for each range of interaction belong to a new universality class which is in sharp contrast to earlier results of the only work that exist on RSBD.

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Chapter 1

Introduction

Percolation is one of the most studied problems in statistical physics. Its idea was first conceived by Paul Flory in the early 1940s in the context of gelation in polymers [53]. Since then it has come a long way holding the hands of respected scientists. Physicists are always interested in describing natural phenomena in a simplified way. Phase transition is one of the most studied problem in physics and using percolation phenomena we can mimic phase transition in real system. Phase transition always includes at least one critical point below which the system behaves in one way and above it the system behaves in a completely different way. For example liquid to gas transition. Phase transition as of two kinds: first order and second order, which is classified in terms of discontinuity of derivatives of thermodynamic potentials. The transitions between solid, liquid and gaseous phases are the examples of first order phase transitions and paramagnetic-ferromagnetic transition, Bose-Einstein condensation [25], superconductivity, superfluidity [80] are some examples of the second order phase transition.

In todays time the definition of transition is given in terms of entropy and order parameter. If we plot entropy versus temperature for a certain transition and if it shows a discontinuity at the critical point, we classify it as a first order transition and continuity is for second order transition. The reason behind this is the fact that first order transition requires latent heat [105] and second order does not. We can definite the type of the transition using order parameter which is a measure of how ordered the system is at a particular temperature. A system is said to be more ordered in the low temperature region and highly disordered or less ordered in the high temperature region. Thus the order parameter is considered as zero

in one phase and non-zero in the other and varies below, at and above the critical point, T_c [107]. One thing we need to understand that a system is almost always disordered at $T > T_c$ phase where there is a higher degree of symmetry in the system. Now the system becomes more ordered in $T < T_c$ phase which is why there must be some kind of symmetry breaking involved. Thus we have both entropy and order parameter to be discontinuous at the critical point. This continuity is followed by a jump in the entropy and parameter due to the involvement of latent heat. Now symmetry may or may not be broken in such transition. But, on the other hand, in second order phase transitions, the order parameter is continuous across the critical point which have made us refer to these transitions as continuous phase transition. Symmetry must be broken for such transitions to occur.

Now it is found that in continuous phase transition order parameter P , specific heat C and susceptibility χ follows power law.

$$P \sim \varepsilon^\beta \quad (1.1)$$

$$C \sim \varepsilon^\alpha \quad (1.2)$$

$$\chi \sim \varepsilon^\gamma \quad (1.3)$$

where

$$\varepsilon \sim (T - T_c) \quad (1.4)$$

and the correlation length

$$\xi \sim \varepsilon^{-\nu} \quad (1.5)$$

Thus these quantities diverges at T_c and the exponents $\alpha, \beta, \gamma, \nu$ are said to be universal and they follow the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$ which reduces to equality under static scaling hypothesis [124]. Many actual experiments and exactly solved models suggest that the Rushbrooke inequality holds as an equality [47] and the observations we made in our research actually provides evidence to it. Thus these exponents are bound by scaling relations no matter what the system is.

Now in percolation we take a lattice (graph) consists of sites and bonds (nodes and link). In bond percolation we pick bonds sequentially and occupy it with probability p and keep

it empty with probability $(1 - p)$. And we visit the entire lattice doing so. For a certain probability p_c there emerges a giant cluster called the spanning cluster which spans the entire lattice. This probability is the critical point and called critical occupation probability p_c . In site percolation we occupy sites and get similar results. The process described here is a very slow algorithm and a better alternative is to use NZ algorithm [97, 98]. The interesting this is that at critical point the order parameter, specific heat and susceptibility follows power law with different exponents. We are interested in finding those exponents mainly.

1.1 Motivation and Objective

Percolation is about 60 years old theory and every now and then it finds it's application in various aspects of science. It is a great model to describe phase transition yet it is a very simple one. Among the different quantities involving phase transition the entropy and order parameter is the one that is of primary focus. But, unlike bond percolation, there arises some conflict with the second law of thermodynamics when we try to understand entropy and order parameter int site percolation. Entropy quantifies the degree of disorder and order parameter that measures the extent of order. The traditional definition of site percolation states that we occupy site and measure cluster size with the number of sits in the cluster. This definition results in a serious violation of the second law of thermodynamics. It also gives ambiguity to the initial states of the system. Solving this problem does not affect the current results of site percolation, it just make it consistent.

The deposition (or adsorption) of large particles on solid surfaces is a subject of considerable practical importance. Examples include proteins, bacteria, viruses, latex, and colloidal particles. The process may be thought of as consisting of two steps: the transport of the particle to the surface and its subsequent adhesion. Both steps are influenced by diverse physical and chemical forces. In the transport step hydrodynamic, diffusional, and, if present, external fields like gravity are dominant. Recent work has focused on the development of statistical mechanical models for the geometrical blocking effect of the preadsorbed particles on the adsorption kinetics and resulting structure of the monolayer. The irreversible nature of the process necessitates the use of nonstandard methods and the analysis of even simple

models is nontrivial. An example of the latter category is the much studied random sequential adsorption (RSA) process [126, 4, 130]. In RSA process we take a surface (say a lattice) and deposit particle (like hard sphere) there sequentially. Each particle cover a certain area and another particle cannot be in that area. Now if a particle is tried to be deposited in the occupied area it is simply rejected. Now what if the particle is not rejected. Instead it hits the particle and rolls down and take it's place in the empty area along side the original particle. This is the main theme behind the our work (the RSBD model [126]) .

Another important point is that in site percolation we only occupy the randomly chosen site which we say a close or short range interaction. But the successful model of phase transition in statistical mechanics, i.e. Ising model, has been studied for long range interaction as well [66, 30]. This gives us idea of long range interaction. We call it Random Sequential Ballistic Deposition or RSBD for short.

Traditionally, in site percolation, so far we have been choosing a site and occupying it without considering the state it's neighbor. If we don't consider the neighbor we have a system with sort range interaction. If we, however, consider the neighbor when occupying sites we get a rather long range interaction. The process is quite simple. We choose a site at random according to NZ algorithm and occupy it if it is empty. If it is already occupied then we choose one of it's neighbor and occupy it if the neighbor is empty and we call it L_1 interaction. But if the neighbor is also occupied by any previous process then we choose the next one in the direction of the first neighbor to occupy if it is empty else we just skip the step and we call it L_2 interaction. Note that L_1 denotes interaction up to first neighbor and L_2 denotes interaction up to 2nd neighbor. We investigate some properties and we find that L_0, L_1, L_2 belongs to their own universality classes.

1.2 Method of Study

The observation for our model was done through computer simulation. We have used C++ language to write a program which generates a virtual lattice with sites and bonds and perform percolation according to the given rules. C++ is used for simulation because we need lots and lots of data and the language is very fast since it is compiled language. Data was generated for 20,000 independent realization. Some of the data we processed using binomial

distribution [98] to get data for canonical ensemble. And then they we analyzed using *python* language because it comes with different types of data analyzing and visualization tools. The codes that are used for generating data is given in Appendix (A) and link for full code is provided there. The code for convolution is given in Appendix (B) and link for it is provided there.

1.3 Organization of Chapters

This thesis consists of five chapters apart from this chapter. We discuss basic tools that we use, e.g. similarity, self-similarity, Buckingham π Theorem, scaling hypothesis and homogeneous functions, in chapter (2). In chapter (3) we discuss basic concepts of phase transition and it's classification and the shapes of thermodynamic quantities and a model that can describe phase transition, i.e. Ising model. In chapter (4) we discuss percolation phenomena and how calculate quantities in percolation. Exact solution is given in this chapter. Then we get to chapter (5) where we have done our work on RSBD model and we describe the process of finding exponents and data collapse and how we get universality classes. Finally in chapter (6) we summarize the results and briefly describe it's significance.

Chapter 2

Scaling, Scale-Invariance and Self-Similarity

In physics we observe a natural phenomena and try to understand it using the existing knowledge. To do this we need to assign numbers to the observable quantities. If we can express it in numbers only then we can say we have acquired some knowledge about that quantity. And if we cannot do this then our knowledge is not complete about that quantity. This reveals the fact that physics is all about observation and measurement of physical quantities with the desire to acquire some knowledge about it and then use that knowledge to predict something that is yet to observe. For example, Albert Einstein predicted the existence of gravitational waves in 1916 in his general theory of relativity and the first direct observation of gravitational waves was made on 14 September 2015 and was announced by the LIGO and Virgo collaborations on 11 February 2016. Now, in order to understand the observation of a natural or artificial phenomena we need some tools. Since here we are trying to understand phase transition, finite size scaling (FSS) hypothesis is a great tool for the investigation. In this chapter we will try to understand the fundamentals which is based on Buckingham π theorem, self similarity and homogeneous functions.

2.1 Dimensions of Physical Quantity

In order to express physical quantities in terms of numbers we need a unit of measurement, since a number times unit tells us how much the quantity is larger or smaller with respect to the unit. The units of measurement are described as fundamental and derivative ones. The fundamental units of measurement are defined arbitrarily in the form of certain standards, while the derivative ones are obtained from the fundamental units of measurement by virtue of the definition of physical quantities, which are always indications of conceptual method of measuring them. An example involving fundamental and derivative unit of measurement is velocity. Since velocity is measured by how much distance an object travels per unit time, the unit of velocity is the ratio of distance or length over time. It is expressed as $[v] = LT^{-1}$, where L is the unit of length and T is the unit of time. The unit of length and time are fundamental here and the unit of velocity is the derivative of these two. A system of units of measurement is a set of fundamental units of measurement sufficient to measure the properties of the class of phenomena under consideration. For example the *CGS* system where length is measurement in terms of centimeter, mass is measured in terms of gram and the *SI* system where the mass is measured in terms of kilogram, length is measured in terms of meter and in both system time is measured in terms of second.

Dimension of physical quantity determines by what amount the numerical value must be changed if we want to go to another system of units of measurement. For instance, if the unit of length is decreased by a factor L and the unit of time is decreased by a factor T , the unit of velocity is smaller by the factor of LT^{-1} than the original unit, so the numerical value of velocity would scaled up by a factor of LT^{-1} owing to the definition of equivalence.

The changes in the numerical values of physical quantities upon passage from one systems of units of measurement to another within the same class are determined by their dimensions. The functions that determines the factor by which the numerical value of a physical quantity changes upon transition from systems of unit of measurement to another system within a given class is called the dimension function or, the dimension of that physical quantity. We emphasize that the dimension of a given physical quantity is different in different classes of systems of units. For example, the dimension of density I in the *MLT* class is $[\rho] = ML^{-3}$ whereas in the *FLT* class it is $[\rho] = FL^{-4}T^{-2}$ [? 111].

2.2 Buckingham π Theorem

A part of physics is about modeling physical phenomenon. And while doing it, the first thing is to identify the relevant variables, and then relate them using known physical laws. For simple phenomenon this task is not hard since it involves deriving some quantitative relationship among the physical variables from the first principles. But when dealing with complex systems we need a systematic way of dealing with the problem of reducing number of parameters. In these situations constructing a model in a systematic manners with minimum input parameters that can help analyzing experimental results has been a useful method. One of the simplest way is based on dimensional analysis. Its function is to reduce a large number of parameters into a manageable set of parameters. Buckingham π theorem is one of the most suitable and studied mathematical process to deal with this kind of problems.

Buckingham π theorem describes dimensionless variables obtained from the power products of governing parameters denoted by Π_1, Π_2, \dots etc. When investigating a certain dimensional physical quantity (governed) that depend on other n dimensional variables then this theorem provide us a systematic way to reduce the degrees of freedom of a function. Using this theorem we reduce a function of n variables problems into a function of k dimensionless variable problem if each of the k dimensional variable of original n variables can be expressed in terms of the $n - k$ dimensionally independent variable [28].

The relationship found in physical theories or experiments can always be represented in the form

$$a = f(a_1, a_2, \dots, a_n) \quad (2.1)$$

where the quantities a_1, a_2, \dots, a_n are called the governing parameters. It is always possible to classify the governing parameters a_i 's into two groups using the definition of the dependent and independent variables. Let the arguments a_{k+1}, \dots, a_n have the independent dimensions and the dimensions of the arguments a_1, a_2, \dots, a_k can be expressed in terms of the dimensions

of the governing independent parameters a_{k+1}, \dots, a_n in the following way

$$\begin{aligned}[a_1] &= [a_{k+1}]^{\alpha_1} \dots [a_n]^{\gamma_1} \\ [a_2] &= [a_{k+1}]^{\alpha_2} \dots [a_n]^{\gamma_2}\end{aligned}\tag{2.2}$$

$$\begin{aligned}&\vdots \\ [a_k] &= [a_{k+1}]^{\alpha_k} \dots [a_n]^{\gamma_k}\end{aligned}\tag{2.3}$$

The dimension of the governed parameter a must also be expressible in terms of the dimensionally independent governing parameters a_1, \dots, a_k since a does not have independent dimension and hence we can write

$$[a] = [a_{k+1}]^{\alpha} \dots [a_n]^{\gamma}\tag{2.4}$$

Thus, there exist number α, γ such that Eqn. (2.4) holds. We have set of governing parameters.

$$\Pi_1 = \frac{a_1}{[a_{k+1}]^{\alpha_1} \dots [a_n]^{\gamma_1}}\tag{2.5}$$

$$\Pi_2 = \frac{a_2}{[a_{k+1}]^{\alpha_2} \dots [a_n]^{\gamma_2}}\tag{2.6}$$

$$\vdots\tag{2.7}$$

$$\Pi_k = \frac{a_k}{[a_{k+1}]^{\alpha_k} \dots [a_n]^{\gamma_k}}\tag{2.8}$$

and a dimensionless governed parameter

$$\begin{aligned}\Pi &= \frac{a}{[a_{k+1}]^{\alpha} \dots [a_n]^{\gamma}} \\ &= \frac{f(\Pi_1, \dots, \Pi_k, a_{k+1}, \dots, a_n)}{[a_{k+1}]^{\alpha} \dots [a_n]^{\gamma}}\end{aligned}\tag{2.9}$$

The right hand side of equation (2.9) clearly reveals that the dimensionless quantity Π is a function of $a_{k+1}, \dots, a_n, \Pi_1, \dots, \Pi_k$, i.e.,

$$\Pi \equiv F(a_{k+1}, \dots, a_n, \Pi_1, \dots, \Pi_k)\tag{2.10}$$

The quantities Π, Π_1, \dots, Π_k are obviously dimensionless, and hence upon transition from one system of unit to another inside a given class their numerical values must remain unchanged. At the same time, according to the above, one can pass to a system of units of measurement such that any of the parameters of a_{k+1}, \dots, a_n , say for example, a_{k+1} , is changed by an arbitrary factor, and the remaining ones are unchanged. Upon such transition the first argument of F is unchanged arbitrarily, and all other arguments of the function remain unchanged as well as its value Π . Hence, it follows $\frac{\delta F}{\delta a_{k+1}} = 0$ and entirely analogously $\frac{\delta F}{\delta a_{k+2}} = 0, \dots, \frac{\delta F}{\delta a_n} = 0$. Therefore, the relation (2.10) is in fact represented by a function of k arguments and proves it is independent of a_{k+1}, \dots, a_n , that is,

$$\Pi = \Phi(\Pi_1, \dots, \Pi_k) \quad (2.11)$$

and the function f can be written in the following special form (by combining (2.9, 2.10, 2.11))

$$f(a_1, \dots, a_k, \dots, a_n) = a_{k+1}^\alpha \dots a_n^\gamma \Phi(\Pi_1, \dots, \Pi_k) \quad (2.12)$$

equation 2.12 is known as the Buckingham Π theorem. It constitutes one of the central statements in dimensional analysis and has great bearings on scaling theory.

2.2.1 An Example

An explicit example using this theorem is needed for better understanding it's application. The simplest example that can describe basic features of Buckingham Π theorem is the area of a right triangle and Pythagorean theorem.

Consider a right triangle where three sides are of size a, b and c and for definiteness, the smaller of its acute angles θ . Assume that we are to measure the area S of the triangle. The area S can be written in the following form

$$S = S(a, b, c) \quad (2.13)$$

However, the definition of two governing parameters a and b can be expressed in terms of c alone since we have

$$[a] \sim [c] \text{ and } [b] \sim [c] \quad (2.14)$$

and so is true for the governed parameter S as we can write the dimensional relation $[S] \sim [c^2]$. We therefore can define two dimensionless parameters

$$\Pi_1 = \sin \theta = a/c \quad (2.15)$$

$$\Pi_2 = \cos \theta = b/c \quad (2.16)$$

and the dimensionless governed parameter

$$\Pi = \frac{S}{c^2} = c^{-2} S(c\Pi_1, c\Pi_2, c) \equiv F(c, \Pi_1, \Pi_2) \quad (2.17)$$

Now it is possible to pass from one unit of measurement to another system of unit of measurement within the same class and upon such transition the arguments Π_1, Π_2 of the function F and the function itself remain unchanged. It implies that the function F is independent of c and hence we can write

$$\Pi = \phi(\Pi_1, \Pi_2) \quad (2.18)$$

However, Π_1 and Π_2 both depends on the dimensionless quantity θ and hence we can write

$$S = c^2 \phi(\theta) \quad (2.19)$$

where the scaling function $\phi(\theta)$ is universal in character. In order to further capture the significance of equation (2.19) we rewrite it as

$$\frac{S}{c^2} \sim \phi(\theta) \quad (2.20)$$

This result has far reaching consequences. For instance, consider that we have a right triangle of any arbitrary sides $a' \neq a$, $b' \neq b$ and $c' \neq c$ but have the same acute angle θ as before. This can be ensured by choosing an arbitrary point on the hypotenuse of the previous triangle and drop a perpendicular on the base b . Consider that the area of the new triangle is S' yet we will have

$$\frac{S}{c^2} = \frac{S'}{(c')^2} \quad (2.21)$$

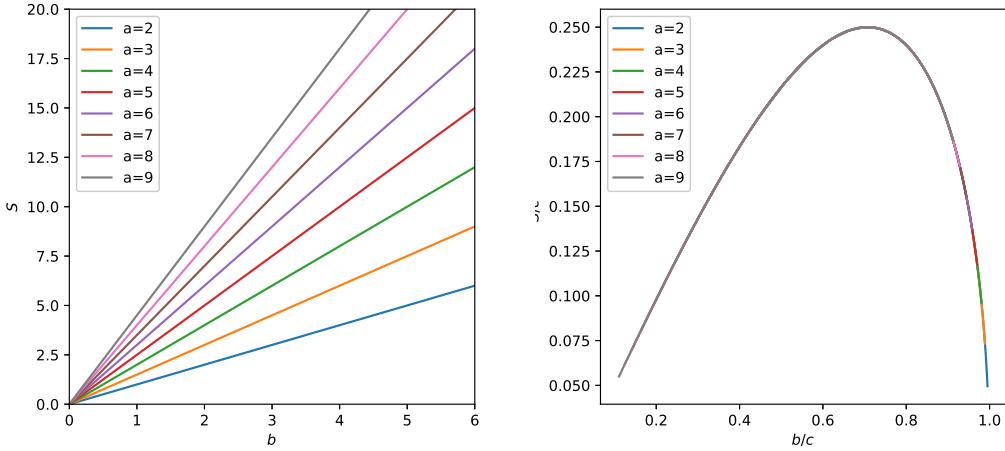
since the numerical value of the ratio of the area over the square of the hypotenuse depends on the angle θ . It implies that if we plot the ratio of the area over the square of the hypotenuse as a function θ all the data points should collapse onto a single curve regardless of the size of the hypotenuse and the respective areas of the right triangle. In fact, the details calculation reveals that

$$\phi(b/c) = \frac{1}{2} \sin \theta \quad (2.22)$$

This data collapse implies that if two or more right triangles which have one of the acute angle identical then such triangles are similar. We shall see later that whenever we will find data collapse between two different systems of the same phenomenon then it would mean that the corresponding systems or their underlying mechanisms are similar. Similarly, if we find that data collected from the whole system collapsed with similarly collected data from a suitably chosen part of the whole system then we can conclude that part is similar to the whole, implying self-similarity. On the other hand, if we have a set of data collected at many different times for a kinetic system and find they all collapse onto a single curve then we can say that the same system at different times are similar. However, similarity in this case is found of the same system at different times and hence we may coin it as temporal self-similarity.

2.3 Similarity and Self-Similarity

The concept of physical similarity is a natural generalization of the concept of similarity in geometry. For instance, two triangles are similar if they differ only in the numerical values of the dimensional parameters, i.e. the lengths of the sides, while the dimensionless parameters, the angles at the vertices are identical for the two triangles. Analogously, physical phenomena are called similar if they differ only in their numerical values of the dimensional governing parameters; the values of the corresponding dimensionless parameters Π_1, \dots, Π_k are being identical. In connection with this definition of similar phenomena, the dimensionless quantities are called similarity parameters. The term *self-similarity* is, as the term itself suggests, a structure or process and a part of it appear to be similar to the whole when compared. This also means that a self-similar structure is infinite in theory. Therefore



(a) S vs b graph. b is the base of the triangle which is varied for a single θ .

(b) S/c^2 vs b/c graph. This each graph contains information about all triangle with a certain acute angle, meaning the entire graph contains information about every right triangle.

Fig. 2.1 Application of Buckingham Π theorem in a right triangle

the fundamental principle of a self-similar structure is the repetition of a unit pattern on different scales.

2.3.1 An example

At this point a real world example will be helpful. Suppose we need to build an airplane. Obviously it's a billion dollar project. If we try to build the airplane directly without first building a prototype then we will waste time, money and man power. Because we can not build an actual working airplane without following certain steps. First we need to build a small-scale model of the airplane. Then we need to test the model for performance. If it is satisfying then we can start building a prototype using the knowledge obtained from the experimentation on the model. Here the model and the prototype are similar to each other. That's why this method works. Since only the dimensional parameters are scaled.

2.3.2 Diving Into Similarity

Let us consider two similar phenomena, one of which will be called the prototype and the other the model. For both phenomena there is some relation of the form

$$\alpha = f(a_1, a_2, a_3, b_1, b_2) \quad (2.23)$$

where the function f is the same for both cases by the definition of similar phenomena, but the numerical values of the governing parameters a_1, a_2, a_3, b_1, b_2 are different. Thus for prototype we have

$$\alpha_p = f(a_1^{(p)}, a_2^{(p)}, a_3^{(p)}, b_1^{(p)}, b_2^{(p)}) \quad (2.24)$$

and for model we have

$$\alpha_m = f(a_1^{(m)}, a_2^{(m)}, a_3^{(m)}, b_1^{(m)}, b_2^{(m)}) \quad (2.25)$$

where the index p denotes quantities related to the prototype and the index m denotes quantities related to the model. Consider that b_1 and b_2 are dependent variable and thus they are expressed in terms of a_1, a_2, a_3 in both model and prototype systems. Using dimensional analysis we find for both phenomena

$$\Pi^{(p)} = \Phi(\Pi_1^{(p)}, \Pi_2^{(p)}) \quad (2.26)$$

and

$$\Pi^{(m)} = \Phi(\Pi_1^{(m)}, \Pi_2^{(m)}) \quad (2.27)$$

where the function Φ must be the same for the model and the prototype. By the definition of similar phenomena the dimensional quantities must be identical in both the cases such as in the prototype and in the model, i.e.,

$$\Pi_1^{(m)} = \Pi_1^{(p)} \quad (2.28)$$

$$\Pi_2^{(m)} = \Pi_2^{(p)} \quad (2.29)$$

It also follows that the governed dimensionless parameter satisfies

$$\Pi^{(m)} = \Pi^{(p)} \quad (2.30)$$

Returning to dimensional variables, we get from the above equation

$$a_p = a_m \left(\frac{a_1^{(p)}}{a_1^{(m)}} \right)^{q_1} \left(\frac{a_2^{(p)}}{a_2^{(m)}} \right)^{q_2} \left(\frac{a_3^{(p)}}{a_3^{(m)}} \right)^{q_3} \quad (2.31)$$

which is a simple rule for recalculating the results of measurements on the similar model for the prototype, for which direct measurement may be difficult to carry out for one reason or another.

The conditions for similarity of the model to the prototype-equality of the similarity parameters Π_1, Π_2 for both phenomena show that it is necessary to choose the governing parameters $b_1^{(m)}, b_2^{(m)}$ of the model as to guarantee the similarity of the model to the prototype

$$b_1^{(m)} = b_1^{(p)} \left(\frac{a_1^{(m)}}{a_1^{(p)}} \right)^{\alpha_1} \left(\frac{a_2^{(m)}}{a_2^{(p)}} \right)^{\beta_1} \left(\frac{a_3^{(m)}}{a_3^{(p)}} \right)^{\gamma_1} \quad (2.32)$$

and

$$b_2^{(m)} = b_2^{(p)} \left(\frac{a_1^{(m)}}{a_1^{(p)}} \right)^{\alpha_2} \left(\frac{a_2^{(m)}}{a_2^{(p)}} \right)^{\beta_2} \left(\frac{a_3^{(m)}}{a_3^{(p)}} \right)^{\gamma_2} \quad (2.33)$$

whereas the model parameters $a_1^{(m)}, a_2^{(m)}, a_3^{(m)}$ can be chosen arbitrarily. The simple definitions and statements presented above describe the entire content of the theory of similarity.

2.3.3 Self-Similarity

A system is called self-similar When a small part of the system is similar to the whole system. A self similar structure is created by repetition of a unit pattern or a simple rule over different size scales [88]. Although the term "self-similarity" itself is explanatory, some example gives better insight.

The cauliflower head contains branches or parts, which when removed and compared with the whole found to be very much the same except it is scaled down. These isolated



(a) A cauliflower

(b) Dissection of cauliflower

Fig. 2.2 Self-Similarity in Cauliflower

branches can again be decomposed into smaller parts, which again look very similar to the whole as well as of the branches. Such self-similarity can easily be carried through for about three to four stages. After that the structures are too small to go for further dissection. Of course, from the mathematical point of view the property of self-similarity may be continued through an infinite stages though in real world such property sustain only a few stages (2.2).

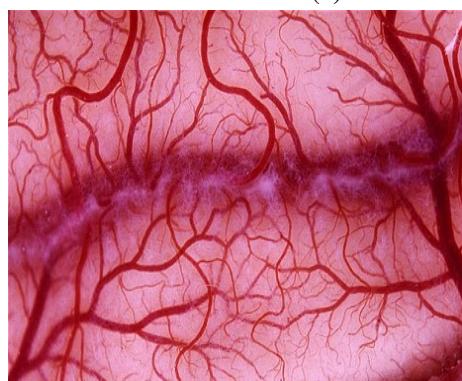
There are plenty of other examples of self similarity in nature. Snowflakes exhibit self-similar branching patterns (2.3). The growth in aggregating colloidal particles are statistically self-similar. A leafless tree branches (2.3) in a self-similar fashion, each length splitting into two or more branches. This branch pattern is repeated on smaller and smaller length scales till the tree top is reached. The veins of the leaves also branch in a self similar manner (2.3). The decimal number system is a construct that uses the idea of self-similarity. If we look a meter stick, we shall see that a decimeter range with its marks looks like a meter range with its marks, only smaller by a factor of 10. This pattern of meter stick makes it very easy to note readings. The human brain is also a complex network of neurons which organize in self-similar patterns. From quantum particle paths, lightning bolts, blood vessels (2.3), aggregation of bacteria all are example of self-similarity.



(a) Leaf



(b) Snowflake



(c) Blood vessel



(d) Leafless Tree

Fig. 2.3 Self-Similarity examples

One thing must be mentioned although it is understandable from the above discussion is that a system is to be called self-similar in the statistical sense even if it is not visible to the eye [87].

2.4 Scaling Hypothesis

2.4.1 Dynamic Scaling

Dynamic scaling (sometimes known as Family-Vicsek scaling [50, 127]) is the litmus test of showing that an evolving system exhibits self-similarity. A function $f(x,t)$ is said to obey dynamic scaling if one of the variable t strictly denotes time and if it satisfies

$$f(x,t) \sim t^\theta \phi(x/t^z) \quad (2.34)$$

where t is independent variable and θ and z are fixed by the dimensional relation $[t^\theta] = [f]$ and $[t^z] = [x]$ respectively, while $\phi(\xi)$ is known as the scaling function. Sometimes it is also written in the following form

$$f(x,t) \sim x^\omega \phi(x/t^z) \quad (2.35)$$

where x is consider independent variable.

Buckingham π -theorem can provide a systematic processing procedure to obtain the dynamic scaling form and at the same time appreciate the fact that the second form is not mathematically sound. An interesting aspect of the structure of the dynamic scaling form given by equation (2.34) is that the distribution function $f(x,t)$ at various moments of time can be obtained from one another by a similarity transformation

$$x \rightarrow \lambda^z x \quad (2.36)$$

$$t \rightarrow \lambda t \quad (2.37)$$

$$f \rightarrow \lambda^\theta \quad (2.38)$$

revealing the self-similar nature of the function $f(x,t)$.

To derive it one has to know first that one of the two governing parameters can be assumed to be independent. Let us assume that t is chosen to be an independent parameter and hence x can be expressed in terms of t

$$x \sim t^z \quad (2.39)$$

It implies that we can choose t^z as unit of measurement or yard-stick and quantify x in terms of dimensionless quantity $\xi = x/t^z$. Here, the quantity ξ is a number that tells how many t^z we need to measure x . If t is independent quantity then we can also express f in units of t^θ to obtain yet another dimensionless quantity $\phi = f(x,t)/t^\theta$ where the exponent θ is fixed by the dimensional requirement $[f] = [t^\theta]$. Since ϕ is a dimensionless quantity its numerical value can only depend on dimensionless quantity ξ not on a dimensional quantity t . We can then immediately obtain the scaling form given by Eq. (2.34). On the other hand, had we choose x to be independent parameter instead of t then following the same argument we would have the following scaling (2.35).

2.4.2 Finite Size Scaling

Finite-size scaling, as formulated by Fisher and Barber [52] concerns itself with the manner in which this rounding or crossover occurs. In a finite-size system, there are in principle three length scales involved: ξ, L and the microscopic length a which governs the range of the interactions. Thermodynamic quantities thus may in principle depend on the dimensionless ratios ξ/a and L/a . The finite-size scaling hypothesis assumes that, close to the critical point, the microscopic length drops out. Thus, if we consider a quantity such as the ferromagnetic susceptibility χ , which behaves like near the critical point in the infinite system, then in the finite geometry characterized by a size L ,

$$\chi = \chi^{\gamma/\nu} \phi(\xi/L) \quad (2.40)$$

Equation of this sorts is used in any phase transition model.

The finite-size scaling (FSS) [5] has been extensively used as a very powerful tool for estimating finite size effects specially in the second order phase transition near the critical temperature T . The various response functions, typically the second derivative of the free energy F , in second order phase transition diverges. Such transitions are clasified by a set of

critical exponents which characterize the critical point. The best known example of second order phase transition is the paramagnetic to ferromagnetic transition where

$$M \sim (T - T_c)^\beta \quad (2.41)$$

$$\chi_M \sim (T - T_c)^{-\gamma} \quad (2.42)$$

$$C_V \sim (T - T_c)^{-\alpha} \quad (2.43)$$

$$\xi \sim (T - T_c)^{-\nu} \quad (2.44)$$

where, M, χ_M, C_V, ξ are Magnetization, Susceptibility, Heat capacity, Correlation length respectively. These relations are only true in the thermodynamic limit in the sense that the system size is infinite. However, we can work in simulation and experiment with finite size L^d where correlation length $\xi \sim L$. Finite size scaling thus provides a means of extrapolating various results for infinite systems.

According to finite size scaling (FSS) hypothesis, a function $f(\varepsilon, L)$ with $\varepsilon = T - T_c$ is said to obey finite size scaling if it can be expressed as

$$f(\varepsilon, L) \sim L^{-\omega/nu} \phi(\varepsilon L^{1/\nu}) \quad (2.45)$$

However, using the Buckingham π -theorem we not only obtain the correct scaling form but we also gain a deeper insight into the problem as it provides a systematic processing procedure. For instance, as we know that the correlation length ξ in the limit $L \rightarrow \infty$ diverges like $\xi \sim \varepsilon^\nu$ near the critical point and it bear the dimension of length. We therefore can either choose L as an independent parameter and measure ξ , i.e., $T - T_c$, in unit of L . Consequently we can measure L in unit of $T - T_c$ assuming it as an independent parameter. Choosing the later case we can define a dimensionless quantity

$$\pi = \frac{L}{\xi} = L(T - T_c)^\nu \quad (2.46)$$

and the corresponding dimensionless governing parameter is

$$\Pi = \frac{f(\varepsilon, L)}{\xi^\omega} = \phi(\pi) \quad (2.47)$$

Following the argument of the π -theorem we can immediately write that

$$f(\varepsilon, L) \sim (T - T_c)^{-\nu\omega} \phi(L(T - T_c)^\nu) \quad (2.48)$$

On the other hand had we chosen L as an independent parameter then the similar treatment would yield

$$f(\varepsilon, L) \sim L^\theta \phi(\{L(T - T_c)^\nu\}^{-1}) \quad (2.49)$$

Till to date neither of the two scaling forms obtained following π theorem are in use in their strict form. Instead, what is done traditionally are as follows. The important point is that if $\pi = L/\xi$ is dimensionless then so is

$$\pi^{1/\nu} = (L/\xi^{1/\nu}) = (T - T_c)L^{1/\nu} \quad (2.50)$$

It also means that we can choose L as independent parameter and express $(T - T_c)$ in unit of $L^{-1/\nu}$ to make the dimensionless quantity coincide with $\pi^{1/\nu}$. Then f too can be expressed in unit of L^θ which according to the prescription of π -theorem we have the following FSS scaling form

$$f(\varepsilon, L) \sim L^\theta \phi((T - T_c)L^{1/\nu}) \quad (2.51)$$

which is the same as the traditional scaling form given by (2.45) if we find θ negative and it is related to the exponent ν via $\theta = -\omega/\nu$.

A quantitative way of interpreting how the experimental data exhibits finite-size scaling is done by invoking the idea of data-collapse method - an idea that goes back to the original observation of Rushbrooke. That is, the values of $f(\varepsilon, L)$ for different system size L can be made to collapse on a single curve if $fL^{\omega/\nu}$ is plotted against $\varepsilon L^{1/\nu}$. It implies that systems of different sizes are all similar that also include system where $L \rightarrow \infty$. The method of data-collapse therefore comes as a powerful means of establishing scaling. It is extensively used to analyze and extract exponents especially from numerical simulations. We shall elucidate it further in the upcoming chapters.

2.5 Homogeneous Functions and Scale-Invariance

In mathematics, a homogeneous function is one with multiplicative scaling behaviour: if all its arguments are multiplied by a factor, then its value is multiplied by some power of this factor.

For example, a homogeneous function of two variables x and y is a real-valued function that satisfies the condition

$$f(\lambda x, \lambda y) = \lambda^k f(x, y) \quad (2.52)$$

for some constant k and all real numbers λ . The constant k is called the degree of homogeneity [6].

2.5.1 One variable function

A function is called scale-invariant or scale-free if it retains its form keeping all its characteristic features intact even if we change the measurement unit or scale. Mathematically, a function $f(r)$ is called scale-invariant or scale-free if it satisfies

$$f(\lambda x) = g(\lambda) f(x) \quad \forall \lambda \quad (2.53)$$

where $g(\lambda)$ is yet unspecified function. That is, one is interested in the shape of $f(\lambda x)$ for some scale factor λ which can be taken to be a length or size rescaling. For instance dimensional functions of physical quantity are always scale-free since they obey power monomial law. It can be rigorously proved that the function that satisfies (2.53) should always have power law of the form $f(x) \sim x^{-\alpha}$.

Let us first set $r = 1$ to obtain $f(\lambda) = g(\lambda)f(1)$. Thus $g(\lambda) = f(\lambda)/f(1)$ and equation (2.53) can be written as

$$f(\lambda x) = \frac{f(\lambda)f(x)}{f(1)} \quad (2.54)$$

The above equation is supposed to be true for any λ , we can therefore differentiate both sides with respect to λ to yield

$$x f'(\lambda x) = \frac{f'(\lambda)f(x)}{f(1)} \quad (2.55)$$

where f' indicates the derivative of f with respect to its argument. Now we set $\lambda = 1$ and get

$$xf'(x) = \frac{f'(1)f(x)}{f(1)} \quad (2.56)$$

This is a first order differential equation which has a solution

$$f(x) = f(1)x^{-\alpha} \quad (2.57)$$

where $\alpha = -f(1)/f'(1)$. There it is proven that the power law is the only solution that can satisfy (2.53). We can also prove that $g(\lambda)$ has a power law form as well.

Power law distribution of the form $f(x) \sim x^{-\alpha}$ are said to be scale free since the ratio $\frac{f(\lambda x)}{f(x)}$ depends on λ alone. Thus the distribution does not need a characteristic scale. If we change the unit of measurement of x by a factor of λ , the numerical value of $f(x)$ will change by a factor of $g(\lambda)$, without affecting the shape of the function f .

2.5.2 Generalized Homogeneous Function

A function $f(x, y)$ of two independent variables x and y is said to be a generalized homogeneous function if for all values of the parameter λ the function $f(x, y)$ satisfies,

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x, y) \quad (2.58)$$

where a, b are arbitrary numbers. In contrast to the homogeneous functions defined in the previous section (2.5.1) generalized homogeneous functions can not be written as $f(\lambda x, \lambda y) = \lambda^p f(x, y)$, because (2.58) can not be generalized any further to the following form,

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x, y) \quad (2.59)$$

choosing $p = 1$ in the above equation yields

$$f(\lambda^{a/p} x, \lambda^{b/p} y) = \lambda f(x, y) \quad (2.60)$$

Similarly an statement converse is also valid and the equation above is no more general than the form in the equation (2.58). Another equivalent form of (2.58) is as follows,

$$f(\lambda x, \lambda^b y) = \lambda^p f(x, y) \quad (2.61)$$

Similarly

$$f(\lambda^a x, \lambda y) = \lambda^p f(x, y) \quad (2.62)$$

Note that there are at least two undetermined parameters a and b for a generalized homogeneous function. Now let us see what happens if we choose $\lambda^a = 1/x$ to set in equation (2.58),

$$f\left(1, \frac{y}{x^{b/a}}\right) = x^{-\frac{p}{a}} \quad (2.63)$$

$$f(x, y) = x^{p/a} f(y/x^{b/a}) \quad (2.64)$$

This combining and hence the simplification of two variables x and y into a single term has far reaching consequence in Widom scaling [79, 70, 111] in the theory of phase transition and critical phenomena.

In Statistical Mechanics we have a hypothesis called widom scaling (names after Benjamin Widom) regarding the free energy of a magnetic system near its critical point which leads to the critical exponents. And becomes no longer independent so that they can be parameterized in terms of two values. The hypothesis can be seen to arise as a natural consequence of the block-spin renormalization procedure, when the block size is chosen to be of the same size as the correlation length [123, 79, 70]. Widom scaling is an example of universality.

Chapter 3

Phase Transition

The term phase transition is generally used to describe the transition between solid, liquid or gaseous states and in some cases the plasma state. It is one of the most studied problems in physics. Phase transition is a process where below a critical point the system behaves in one way whereas above that point the system behaves in a completely different way. There is a control parameter in phase transition. It can be temperature T or magnetic field H . For example in ferromagnet to paramagnet transition temperature is the control parameter and for normal to superconductor transition both temperature and magnetic field are the control parameter.

3.1 Classification

3.1.1 Ehrenfest classification

Paul Ehrenfest classified phase transitions based on the behavior of the thermodynamic free energy as a function of other thermodynamic variables [73]. Under this scheme, phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition.

First-order phase transitions exhibit a discontinuity in the first derivative of the free energy with respect to some thermodynamic variable [21]. The various solid/liquid/gas transitions are classified as first-order transitions because they involve a discontinuous change in density, which is the (inverse of the) first derivative of the free energy with respect to pressure.

Second-order phase transitions are continuous in the first derivative (the order parameter, which is the first derivative of the free energy with respect to the external field, is continuous across the transition) but exhibit discontinuity in a second derivative of the free energy [21]. These include the ferromagnetic phase transition in materials such as iron, where the magnetization, which is the first derivative of the free energy with respect to the applied magnetic field strength, increases continuously from zero as the temperature is lowered below the Curie temperature. The magnetic susceptibility, the second derivative of the free energy with the field, changes discontinuously. Under the Ehrenfest classification scheme, there could in principle be third, fourth, and higher-order phase transitions.

Though useful, Ehrenfest's classification has been found to be an incomplete method of classifying phase transitions, for it does not take into account the case where a derivative of free energy diverges (which is only possible in the thermodynamic limit). For instance, in the ferromagnetic transition, the heat capacity diverges to infinity. The same phenomenon is also seen in superconducting phase transition.

3.1.2 Modern classifications

In the modern classification scheme, phase transitions are divided into two broad categories, named similarly to the Ehrenfest classes:[73]

First-order phase transitions are those that involve a latent heat. During such a transition, a system either absorbs or releases a fixed (and typically large) amount of energy per volume. During this process, the temperature of the system will stay constant as heat is added: the system is in a "mixed-phase regime" in which some parts of the system have completed the transition and others have not. Familiar examples are the melting of ice or the boiling of water (the water does not instantly turn into vapor, but forms a turbulent mixture of liquid water and vapor bubbles).

Second-order phase transitions are also called continuous phase transitions. They are characterized by a divergent susceptibility, an infinite correlation length, and a power-law decay of correlations near criticality. Examples of second-order phase transitions are the ferromagnetic transition, superconducting transition (for a Type-I superconductor the phase transition is second-order at zero external field and for a Type-II superconductor the phase transition is second-order for both normal-state—mixed-state and mixed-state—superconducting-state

transitions) and the superfluid transition. In contrast to viscosity, thermal expansion and heat capacity of amorphous materials show a relatively sudden change at the glass transition temperature [101] which enables accurate detection using differential scanning calorimetry measurements

3.1.3 Basic Properties of the classes

Some basic properties of the two classes of phase transition is listed below.

First Order

1. Latent heat of nucleation in growth
2. Symmetry may or may not be broken
3. Discontinuous change in entropy

Second Order

1. No Latent heat or meta-stable state
2. Symmetry is always broken
3. Continuous change in entropy

At the event of critical point of phase transition there might exists a meta-stable state, where both phases exists simultaneously. At the meta-stable state the control parameter or temperature (in case of thermal phase transition, e.g., ice to water or water to vapor) does not change but there is a change (usually large) in heat which give rise to discontinuity of the first derivative of free energy, i.e., entropy (3.2.1, 4.6.3). And if the entropy is continuous then the latent heat is zero which is the signature of second order transition.

3.2 Thermodynamic Quantities

The first explicit statement of the first law of thermodynamics, by *Rudolf Clausius* in 1850, referred to cyclic thermodynamic processes.

In all cases in which work is produced by the agency of heat, a quantity of heat is consumed which is proportional to the work done; and conversely, by the expenditure of an equal quantity of work an equal quantity of heat is produced.

$$\Delta E = Q + W \quad (3.1)$$

where, Q is the net quantity of heat supplied to the system by its surroundings and W is the net work done by the system. The IUPAC convention for the sign is as follows: All net energy transferred to the system is positive and net energy transferred from the system is negative. Clausius also stated the law in another form, referring to the existence of a function of state of the system, the internal energy, and expressed it in terms of a differential equation for the increments of a thermodynamic process.

In a thermodynamic process involving a closed system, the increment in the internal energy is equal to the difference between the heat accumulated by the system and the work done by it.

For quasi-static process

$$dU = \delta Q - \delta W \quad (3.2)$$

$$= dQ - PdV \quad (3.3)$$

U is the internal energy. here $W = -PdV$ since work done by the system on the environment if the product PdV whereas the work done on the system is $-PdV$ for pressure P and volume change dV .

The term heat for Q means "that amount of energy added or removed by conduction of heat or by thermal radiation", rather than referring to a form of energy within the system. The internal energy is a mathematical abstraction that keeps account of the exchanges of energy that befall the system.

For quasi-static state we can write

$$dQ = TdS \quad (3.4)$$

where S is the entropy of the system and T is the temperature. Thus we can write for canonical ensemble

$$dU = TdS - PdV \quad (3.5)$$

such that $E = E(S, V)$ and for grand canonical ensemble

$$dU = TdS - PdV + \mu dN \quad (3.6)$$

where $U = U(S, V, N)$. But a problem arises, since there is no device we currently possess that can measure entropy. So we use Legendre transformation to change variable dependency

$$\begin{aligned} dU &= TdS - PdV \\ &= TdS + SdT - SdT - PdV \\ d(U - TS) &= -SdT - PdV \\ dA &= -SdT - PdV \end{aligned} \quad (3.7)$$

where $A = A(T, V)$ is the Helmholtz free energy. We can perform another Legendre transformation in (3.7) as follows

$$\begin{aligned} dA &= -SdT - PdV - VdP + VdP \\ d(A + PV) &= -SdT + VdP \\ dG &= -SdT + VdP \end{aligned} \quad (3.8)$$

where $G = G(T, P)$ is the Gibbs free energy.

3.2.1 Entropy

One of the most important concept in Statistical Mechanics is entropy. The notion of entropy was first introduced in physics by a German scientist Rudolf Clausius who laid the foundation for the second law of thermodynamics in 1850 by examining the relation between heat transfer and work. The second law of thermodynamics states that the total entropy of an isolated system can never decrease over time. Therefore the direction toward which entropy increases monotonically is the direction of time. Monotonically means that it can increase

or keep constant but never decrease. The term entropy is used in many other branches of science, sometimes distant from physics or mathematics (such as sociology), where it no longer maintains its rigorous quantitative character. Usually, it roughly means disorder, chaos, decay of diversity or tendency toward uniform distribution of kinds [44].

Entropy is considered as a quantity about the disorderness of a system. This kind of disorder is the number of states a system can take on. So what are the states of a system? Imagine a cube of volume 1cm^3 , filled with one particular gas. At a particular time if we can label all the molecules of the gas uniquely then at next moment most of the molecule will change their positions due to their random motion. Then we will not be able to identify each molecule with their previous label. This process of identifying the labels of the molecules are easier if it's a liquid and even more easier in it's solid form. Since temperature increases the random motion of the molecules, as the temperature rises it is more difficult to identify those molecules. Thus at high temperature a system has higher entropy. Another thing to mention about it's volume. If a larger volume is selected then obviously the number of possible states will increase therefore entropy will increase.

Example If we were to compare the entropy of the moon and the sun, the above discussion tells us that the sun has higher entropy than the moon. The reason is that the sun is much much larger than the moon and has much higher temperature than the moon. Therefor the number of possible states will be larger for the sun than the moon.

In Classical Physics, entropy is seen as a magnitude which in every time is proportional to the quantity of energy that at that time cannot be transformed into mechanical work. Using the above interpretation, entropy plays a central role in the formulation of the second law of thermodynamics which states that in an isolated physical system, any transformation leads to an increase of its entropy.

In Probability Theory, the entropy of a random variable measures the uncertainty over the values which can be reached by the variable.

In Information Theory, the entropy of the compression of a message (for example, of a file from a computer), quantifies the content of the information of the message to have the minimum lost of information in the compression process previous to its transmission.

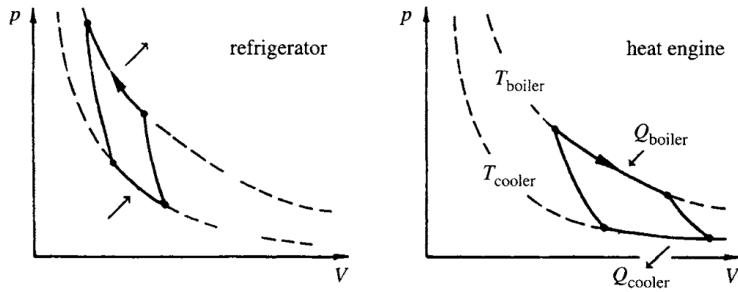


Fig. 3.1 Two competing Carnot engines, pressure (P) versus volume (V) - diagrams [12]

In Abstract Theory of Dynamical Systems, the entropy measures the exponential complexity of the system or the average flow of information per unit of time [14].

So it is already explicit that the concept of entropy is not easy to grasp and frequently entropy is seen as very mysterious quantity and that's why it received a very large number of interpretations, explications, applications. In order to understand how the complex concept of entropy emerged, in this chapter we will give a brief history and will review the works of Clausius, Boltzmann, Shannon and Rényi.

Clausius Entropy

As mentioned Earlier in this section The concept and name of entropy originated in the early 1850s in the work of Rudolf Julius Emmanuel Clausius (1822 – 1888) and that work was at first primarily concerned with the question of which cycle is best suited for the conversion of heat into work and which substance is best used for the conversion [36].

Clausius based his argument on the plausible axiom that heat cannot pass by itself from a cold to a hot body. In order to exploit that axiom Clausius considered two competing Carnot cycles (see figure (3.1)) working in the same temperature range, one as a heat engine and one as a refrigerator; the refrigerator consumes the work the engine provides. By comparing the amounts of heat Q passed from top to bottom and vice versa, he came to the conclusion that among all efficiencies the efficiency of a Carnot cycle is maximum and universal. 'Maximum' means that no cycle in the same range of temperature has a bigger efficiency than a Carnot cycle, and 'universal' means that all working substances provide the same efficiency in a Carnot cycle [32]. It is easy to calculate the efficiency of the Carnot engine of an ideal gas:

$$\begin{aligned}\eta &= \frac{W}{Q_{boiler}} \\ &= \frac{Q_{boiler} - Q_{cooler}}{Q_{boiler}} \\ &= 1 - \frac{Q_{cooler}}{Q_{boiler}} \\ &= 1 - \frac{T_{cooler}}{T_{boiler}}\end{aligned}\tag{3.9}$$

where T is the Kelvin temperature. And, since by Clausius's result this efficiency is universal, it holds not only for ideal gases but for all substances, be they water, mercury, sulphur, or steel. Nicolas Léonard Sadi Carnot anticipated Clausius by 30 years, but no one could understand Carnot's reasoning. Carnot believed in the caloric theory of heat, by which the heat passing through the cycle from boiler to cooler is unchanged in amount. This is quite wrong and it is a kind of miracle that Carnot, despite his erroneous concepts, obtained a correct result. Carnot's trouble was that he did not know the balance of energy, or the first law of thermodynamics, which states that

$$dU = dQ - dW \tag{3.11}$$

$$= dQ - PdV \tag{3.12}$$

since

$$dW = PdV \tag{3.13}$$

This equation holds, if the work is expended reversibly for the volume change. With that superior knowledge Clausius showed that it is not the heat that passes through the cycle from boiler to cooler unchanged in amount. He proved that from equation (3.10)

$$\left. \frac{Q}{T} \right|_{boiler} = \left. \frac{Q}{T} \right|_{heater} \tag{3.14}$$

and decided to define the entropy change to be the ratio of heat flow to temperature: [120]

$$\Delta S_{\text{thermo}} = \frac{Q}{T} \tag{3.15}$$

He also showed that in an arbitrary process, the change of entropy, satisfies the inequality

$$dS \geq \frac{dQ}{T} \quad (3.16)$$

This important relation is known as the second law of thermodynamics. We will now discuss the significance of this law. First, we stick to reversible process, where the equality holds in equation (3.16). We may then eliminate dQ between the first and second laws, we obtain the Gibbs equation

$$dS = \frac{1}{T} (dU + PdV) \quad (3.17)$$

In an adiabatic irreversible process, $dQ = 0$ and equation (3.16) one has the fundamental relation between entropy and irreversibility. In words

In a closed system (adiabatic), the entropy cannot decrease, it remains constant or increase [17]

But the irreversible increase of entropy is not a property of the microscopic laws of nature. Because the microscopic laws of nature are time-reversal invariant. For example the Maxwell's equations are time reversible or the laws governing the motion of electrons of atoms are also time reversible. Thus the direction of time cannot be determined from microscopic laws of nature. But since entropy always increase monotonically, the direction in which entropy increases (or remains constant) is the direction of time [120].

Also by differentiating equation (3.8) with respect to T keeping P constant we can get an expression for entropy in terms of the Gibbs free energy.

$$S = -\frac{dG}{dT} \quad (3.18)$$

similar expression is obtained from (3.7). Thus entropy is indeed the first derivative of free energy with respect to the control parameter T .

Boltzmann Entropy

Another intuitive interpretation of entropy is as a measure of the disorder in a system. Liquids have higher entropy than crystals intuitively because their atomic positions are less orderly [120]. Ludwig Boltzmann interpreted the entropy function as statistical entropy

using probability theory. Around 1900 there was a fierce debate going on between scientists whether atoms really existed or not. Boltzmann was convinced that they existed and realized that models that relied on atoms and molecules and their energy distribution and their speed and momentum, could be of great help to understand physical phenomena. Because atoms were supposed to be very small, even in relatively small systems, one faces already a tremendous number of atoms. For example: one mole of water contains about 6.023×10^{23} molecules! Clearly it is impossible to track the energy and velocity of each individual atom. Therefore, Boltzmann introduced a mathematical treatment using statistical mechanical methods to describe the properties of a given physical system (for example the relationship between temperature, pressure and volume of one liter of air).

Boltzmann's idea behind statistical mechanics was to describe the properties of matter from the mechanical properties of atoms or molecules. In doing so, he was finally able to derive the Second Law of Thermodynamics around 1890 and showed the relationship between the atomic properties and the value of the entropy for a given system. It was Max Planck who formulated the expression of entropy of the ideal gas system based on Boltzmann's results [115]. The Boltzmann entropy formula or Boltzmann-Planck entropy formula is

$$S = k_B \log \Omega \quad (3.19)$$

S is called the Planck entropy or Boltzmann entropy. Here k_B is the Boltzmann constant (ideal gas constant R divided by Avogadro's number N) which equals to $1.4 \times 10^{-23} \text{ J/K}$, and Ω , comes from the German *Wahrscheinlichkeit*, meaning probability, which is often referred to as disorder. In another way we can define it as the number of microstates (often modeled as quantum states) with the given macrostate. Macrostate is any particular arrangement of atoms where we look only on average quantities. Any individual arrangement defining the properties (e.g. positions and velocities) of all the atoms for a given macrostate is a microstate. For a microstate it matters what individual particles do, for the macrostate it does not.

The logarithm is used because it simplifies the computations and reproduced the property of additivity of entropy, in the sense that the entropy of two systems sums instead of multiplies. In equation (3.19), the entropy S increases when Ω increases. More microstates give raise to more disorder hence higher entropy. Besides for only one possible microstate, entropy is

zero. The notion of disorder is an intuitive notion depending of the system to be considered. In the case of a gas, it is considered it in a ordered state if its molecules have a distribution of energies or positions very different of those random which means the Boltzmann distribution. The most disordered states are the most probable and as consequence have the most entropy. Another consequence is that in the universe the disorder tends to increase [14].

From there, it is a short conceptual jump to the second Law (total entropy tends to increase, and all spontaneous processes increase entropy). In summary, the thermodynamic definition of entropy provides the experimental definition of entropy, while the probabilistic definition of entropy extends the concept, providing an explanation and a deeper understanding of its nature [10].

These definitions of entropy is of no use in our model. However we can use the Boltzmann entropy with a few modification to get Shannon entropy [121]. This process of getting Shannon entropy from Boltzmann entropy and how does it help us is described in section (4.6.3).

3.2.2 Specific Heat

Heat capacity is a physical quantity which is the ratio of the heat added to an object to the resulting temperature change [61]. Note that removing heat is just like adding negative heat. The unit of heat capacity if joule per kelvin J/K . And it's dimensional form is $L^2MT^{-2}\Theta^{-1}$. The specific heat is the amount of heat per unit mass ($1kg$) required to raise the temperature by one kelvin($1K$).

Heat capacity is an *extensive* property of matter (it is proportional to the size of the system). When expressing the same phenomenon as an *intensive* property, the heat capacity is divided by the amount of substance, mass, or volume, thus the quantity is independent of the size or extent of the sample. The molar heat capacity is the heat capacity per unit amount (SI unit: mole) of a pure substance, and the specific heat capacity, often called simply specific heat, is the heat capacity per unit mass of a material. In some engineering contexts, the volumetric heat capacity is used.

Temperature represents the average randomized kinetic energy of constituent particles of matter relative to the centre of mass of the system, while heat is the transfer of energy across a system boundary into the body other than by work or matter transfer. Translation,

rotation, and vibration of atoms represent the degrees of freedom of motion which classically contribute to the heat capacity of gases, while only vibrations are needed to describe the heat capacities of most solids, as shown by the Dulong–Petit law [77].

The internal energy of a closed system changes by adding heat to the system or by the system performing work.

$$\Delta E_{\text{system}} = E_{\text{in}} - E_{\text{out}} \quad (3.20)$$

which is same expression as (3.2). If the heat is added at constant volume, then the second term of this relation vanishes to give

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = \left(\frac{\partial Q}{\partial T} \right)_V \quad (3.21)$$

Another useful quantity is the heat capacity at constant pressure, C_P . This quantity refers to the change in the enthalpy of the system given by

$$H = U + PV \quad (3.22)$$

Thus the change in enthalpy is

$$\begin{aligned} dH &= dU + d(PV) \\ &= dQ + dW + PdV + VdP \\ &= dQ + VdP \end{aligned} \quad (3.23)$$

Therefore at constant pressure we have

$$C_P = \left(\frac{\partial H}{\partial T} \right)_P = \left(\frac{\partial Q}{\partial T} \right)_P \quad (3.24)$$

In general we can write the relationship between heat and temperature change as

$$C = \frac{Q}{dT} \quad (3.25)$$

where C is the specific heat. and we know

$$Q = TdS \quad (3.26)$$

we immediately get

$$C = T \frac{dS}{dT} \quad (3.27)$$

Specific heat is called the response function for a non-magnetic system.

3.2.3 Order Parameter

An order parameter is a measure of the degree of order across the boundaries in a phase transition system. It's numerical usually ranges between $[0, 1]$. At the critical point, the order parameter susceptibility will usually diverge.

An example of an order parameter is the net magnetization in a ferromagnetic system undergoing a phase transition. For liquid-gas transitions, the order parameter is the difference of the densities.

Order parameter does have a theoretical perspective. It arise from symmetry breaking. When this happens, one needs to introduce one or more extra variables to describe the state of the system. For example, in the ferromagnetic phase, one must provide the net magnetization, whose direction was spontaneously chosen when the system cooled below the Curie point. Order parameter can be a function of more than one variable. In other words it can have more than one degree of freedom. It can also be defined for non-symmetry-breaking transitions.

3.2.4 Susceptibility

The first law of thermodynamics for a non magnetic system is obtainable from (3.5) using a conversion. For a magnetic system $P \rightarrow h$ and $V \rightarrow -m$, where h is the magnetic field and m is the magnetization. The negative sign for the magnetization is because of the fact that the magnetization increases with the increase of the magnetic field whereas the volume decreases as the pressure increases. Since we relate pressure to the magnetic field, to relate

volume to magnetization we need to put a minus sign with it. Thus we get

$$dU = TdS + hdm \quad (3.28)$$

$$= TdS + SdT - SdT + hdm \quad (3.29)$$

$$d(U - TS) = -SdT + hdm \quad (3.30)$$

$$dA = -SdT + hdm \quad (3.31)$$

$$dA = -SdT + hdm + mdh - mdh \quad (3.32)$$

$$d(A - mh) = -SdT - mdh \quad (3.33)$$

$$dG = -SdT - mdh \quad (3.34)$$

where $A = A(T, m)$ is the Helmholtz free energy and $G = G(T, h)$ is the Gibbs free energy for the magnetic system. From the definition of free energy for a magnetic system (3.34, 3.31) we can find the expression for entropy and magnetization in terms of free energy.

$$S = - \left(\frac{\partial G}{\partial T} \right)_h = - \left(\frac{\partial A}{\partial T} \right)_m \quad (3.35)$$

$$m = - \left(\frac{\partial G}{\partial h} \right)_T \quad (3.36)$$

$$h = \left(\frac{\partial A}{\partial m} \right)_T \quad (3.37)$$

And since the susceptibility is defined as the derivative of the magnetization with respect to the magnetic field, we get

$$\chi = \left(\frac{\partial m}{\partial h} \right)_h = - \left(\frac{\partial^2 G}{\partial h^2} \right)_T \quad (3.38)$$

again we can write χ as

$$\begin{aligned} \chi &= \frac{1}{\frac{\partial h}{\partial m}} \\ &= \frac{1}{\frac{\partial^2 A}{\partial m^2}} \end{aligned} \quad (3.39)$$

Susceptibility is called the response function for a magnetic system.

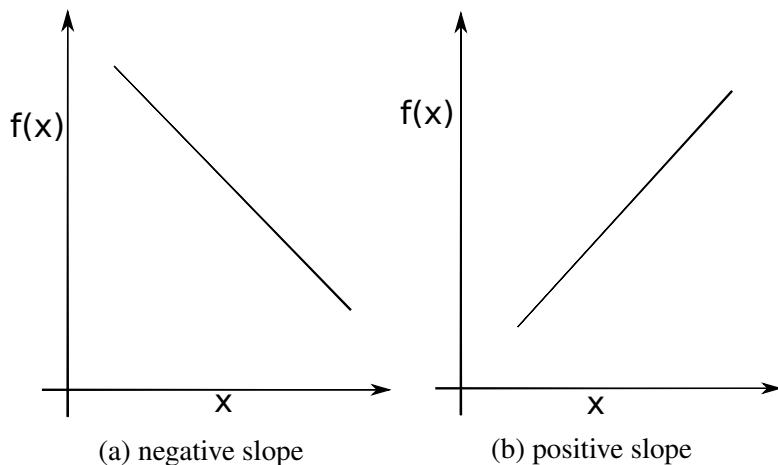


Fig. 3.2 shape of $f(x)$ from $f'(x)$

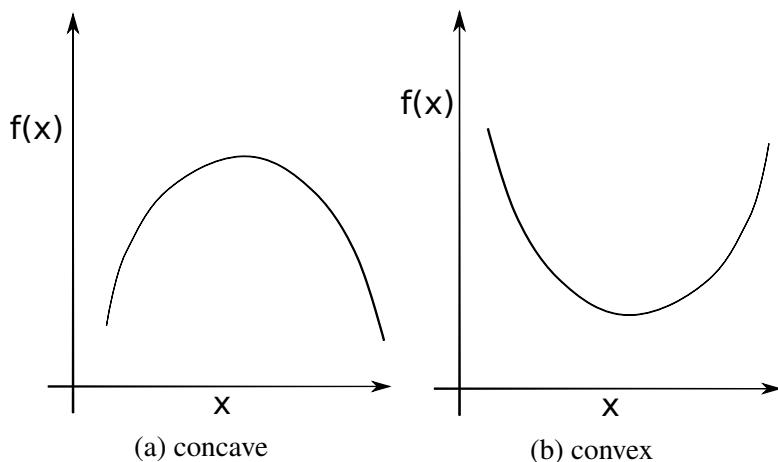


Fig. 3.3 shape of $f(x)$ from $f''(x)$

3.3 Shapes of the Thermodynamic Quantities

3.3.1 Calculus to determine the shapes

From the law of Calculus we can estimate the approximate shape of a function by it's first and second derivative. Say we have a function $f(x)$ and we want to estimate it's shape. If the first derivative of this function is negative (positive) the function is said to have decreasing (increasing) slope (3.2).

If the second derivative of this function is negative (positive) the function is said to have concave (convex) shape (3.3). Thus if we know the sign of the first and second derivative we can approximate a shape of the function.

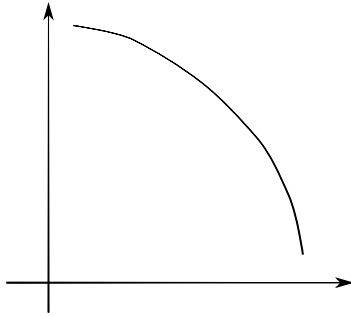


Fig. 3.4 Shape of the free energy

3.3.2 Free Energy

Now since we obtain from (3.8) that the entropy is the first derivative of the free energy (3.40) and from (??) specific heat is the second derivative of the free energy (3.41). Since the entropy is a positive quantity and specific heat is also a positive quantity we get that the first and second derivative of the free energy is negative which implies from the laws of calculus that the shape of the free energy should be a decreasing concave curve (3.4) in other words concave shaped with negative slope.

$$S = -\frac{\partial G}{\partial T} \quad (3.40)$$

$$C = -\frac{\partial^2 G}{\partial T^2} \quad (3.41)$$

3.3.3 Entropy and Specific Heat

Now that we know the shapes of the free energy, the very next thing to do is to find the shape of the entropy. Since we can get entropy from differentiating the free energy with respect to temperature T we get the following shape (3.5). From the definition of the transition order we know that the first order transition is discontinuous and the second order transition continuous. Since the first order transition requires latent heat at the critical point the discontinuity is inevitable. Note that, since entropy measures disorderedness of a system it should increase with increasing temperature. Because the temperature is nothing but the average kinetic energy of the particles in the system. As the kinetic energy of the system increases with

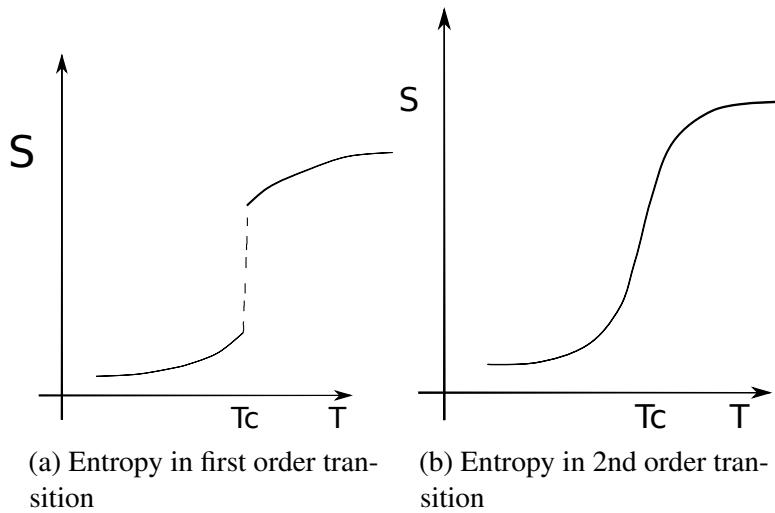


Fig. 3.5 Shape of entropy

temperature, the particles tend to vibrate more and get higher average velocity. Thus making the system disordered. Therefore in a physical system entropy always increases with the increasing of temperature. If we find something different, as if, the entropy is decreasing with the increasing of temperature, there must be a problem somewhere. Just after knowing the shape of entropy one can anticipate the shape of specific heat, which is the derivative of the entropy with respect to temperature and is defined in (??). Using this and the shape of entropy we can get the shape of the specific heat immediately as in figure (3.6)

3.3.4 Order Parameter and Susceptibility

Since diamagnetic substances have negative susceptibilities ($\chi < 0$); paramagnetic, and ferromagnetic substances have positive susceptibilities ($\chi > 0$), and we are working for a phase transition model similar to paramagnet and ferromagnet transition, taking susceptibility to be positive is appropriate for our model. Now if susceptibility is positive then from (3.38) we get $\left(\frac{\partial^2 G}{\partial h^2}\right) < 0$ which means that the shape of the free energy for this case is concave from the knowledge of (3.3.1). And from (3.36) and the fact that the magnetic field h can be positive or negative, as it can change direction, the Gibbs free energy is negative, since it is the lowest binding energy.

Also from (3.39) we can say $\frac{\partial^2 A}{\partial m^2}$ is positive giving convex shape of the Helmholtz free energy.

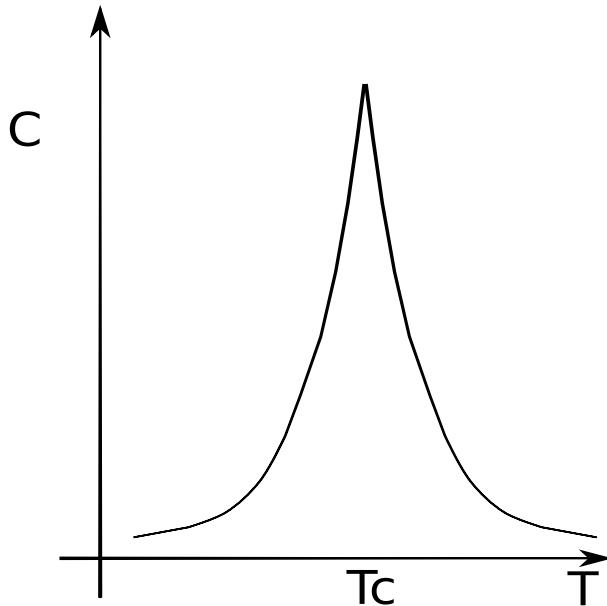


Fig. 3.6 Shape of Specific Heat and Susceptibility

And (3.37) tells us that since h can be positive or negative, the Helmholtz free energy can have increasing or decreasing slope respectively.

3.4 Critical Exponents

Near the critical point there is, in general, a function that describes the behavior of the system that is mostly interesting. For thermodynamical system the temperature is the control parameter , thus that function depends on the temperature. But since we want the information at the critical point, $(T - T_c)/T_c$, instead of T is a better parameter to address. In equation

$$\varepsilon = \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1 \quad (3.42)$$

ε is considered a better parameter. Thus a function $f(\varepsilon)$ is used instead of $f(T)$. Using the fact that in the vicinity of T_c the function $f(\varepsilon)$ exhibits power law

$$f(\varepsilon) \sim \varepsilon^\lambda \quad (3.43)$$

The following figures shows some function that exhibit power law To see this more closely,

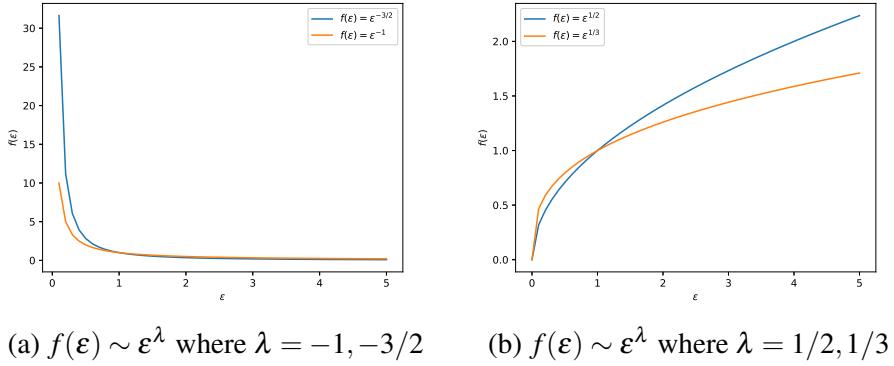


Fig. 3.7 Function showing power law

we can expand any function $f(\varepsilon)$ as a power series of ε

$$f(\varepsilon) = A\varepsilon^\lambda(1 + B\varepsilon^a + C\varepsilon^b + \dots) \quad (3.44)$$

Near T_c only the first term is dominating. We had the Gibbs free energy (for a magnetic system)

$$G = G(T, h) \equiv G(\varepsilon, h) \quad (3.45)$$

since ε is a better parameter. Assuming that G is a generalized Homogeneous function. Therefore from the realization of section (2.5) we can write

$$G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) = \lambda G(\varepsilon, h) \quad (3.46)$$

differentiating equation (3.46) with respect to h

$$\begin{aligned} \frac{\partial G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\partial h} &= \lambda \frac{\partial G(\varepsilon, h)}{\partial h} \\ \frac{\partial G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\partial \lambda^{a_h}h} \lambda^{a_h} &= \lambda \frac{\partial G(\varepsilon, h)}{\partial h} \\ \lambda^{a_h} G'(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda G'(\varepsilon, h) \\ -\lambda^{a_h} m(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= -\lambda m(\varepsilon, h) \\ m(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda^{1-a_h} m(\varepsilon, h) \end{aligned} \quad (3.47)$$

$$(3.48)$$

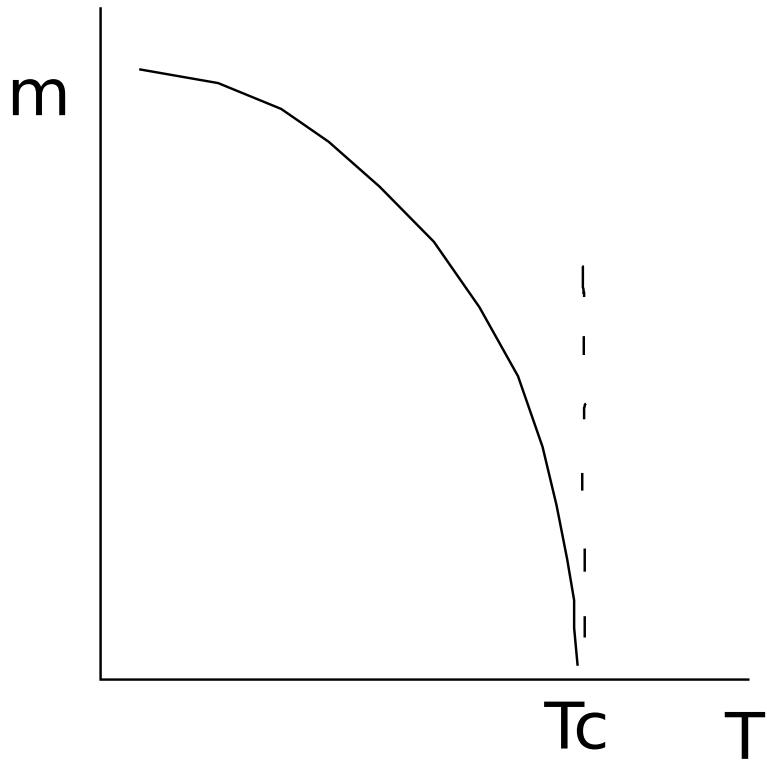


Fig. 3.8 General shape of Order Parameter

Here m is the magnetization or order parameter. The figure (3.8) shows the general shape of the order parameter.

Setting $h = 0$ in equation (3.48)

$$\begin{aligned}
 m(\lambda^{a_\varepsilon} \varepsilon) &= \lambda^{1-a_h} m(\varepsilon) \\
 m(1) &= \lambda^{1-a_h} m(\varepsilon) \\
 m(1) &= \varepsilon^{-\frac{1-a_h}{a_\varepsilon}} m(\varepsilon) \\
 m(\varepsilon) &= \varepsilon^\beta m(1)
 \end{aligned} \tag{3.49}$$

where

$$\beta = \frac{1-a_h}{a_\varepsilon} \tag{3.50}$$

Note that, setting $\lambda^{a_\varepsilon} \varepsilon = 1$ gives $\lambda = \varepsilon^{-1/a_\varepsilon}$.

Setting $\varepsilon = 0$ in equation (3.48)

$$\begin{aligned} m(\lambda^{a_h} h) &= \lambda^{1-a_h} m(h) \\ m(1) &= h^{-\frac{1-a_h}{a_h}} m(h) \\ m(h) &= m(1) h^\delta \end{aligned} \quad (3.51)$$

where

$$\delta = \frac{a_h}{1 - a_h} \quad (3.52)$$

Again, note that, setting $\lambda^{a_h} h = 1$ gives $\lambda = h^{-1/a_h}$

Now, Since the response functions are the second derivative of the free energy (??), by differentiating (3.46) twice with respect to ε we get the Specific Heat

$$\begin{aligned} \lambda^{2a_\varepsilon} G''(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_h} h) &= \lambda G''(\varepsilon, h) \\ \lambda^{2a_\varepsilon} \frac{\partial G(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_h} h)}{\left(\frac{1}{T_c}\right)^2 \partial T^2} &= \lambda G''(\varepsilon, h) \\ \lambda^{2a_\varepsilon} C(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_h} h) &= \lambda C(\varepsilon, h) \end{aligned} \quad (3.53)$$

We have used $\varepsilon = \frac{T}{T_c} - 1$ and $d\varepsilon = \frac{1}{T_c} dT$. Now setting $h = 0$ we get from (3.53)

$$\begin{aligned} \lambda^{2a_\varepsilon} C(\lambda^{a_\varepsilon} \varepsilon) &= \lambda C(\varepsilon) \\ C(1) &= \lambda^{1-2a_\varepsilon} C(\varepsilon) \\ &= \varepsilon^{-\frac{1-2a_\varepsilon}{a_\varepsilon}} C(\varepsilon) \\ C(\varepsilon) &= \varepsilon^{-\alpha} C(1) \end{aligned} \quad (3.54)$$

We have used the value of λ when we set $\varepsilon \lambda^{a_\varepsilon} = 1$ and the exponent

$$\alpha = \frac{2a_\varepsilon - 1}{a_\varepsilon} \quad (3.55)$$

Again by differentiating (3.46) twice with respect to h we get the susceptibility. Then we set $h = 0$ to get only ε dependency.

$$\begin{aligned} \lambda \frac{\partial^2 G(\varepsilon, h)}{\partial h^2} &= \lambda^{2a_h} \frac{\partial^2 G(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_h} h)}{\partial h^2} \\ \lambda \chi(\varepsilon, h) &= \lambda^{2a_h} \chi(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_h} h) \\ \chi(\varepsilon) &= \lambda^{2a_h - 1} \chi(\lambda^{a_\varepsilon} \varepsilon) \\ \chi(\varepsilon) &= \varepsilon^{-\gamma} \chi(1) \end{aligned} \quad (3.56)$$

Similar to previous case, We have used the value of λ when we set $\varepsilon \lambda^{a_\varepsilon} = 1$ and the exponent is

$$\gamma = \frac{2a_h - 1}{a_\varepsilon} \quad (3.57)$$

3.4.1 List of Thermodynamic Quantities that Follows Power Law

The exponent that scales Specific heat is called α

$$C \sim \varepsilon^{-\alpha} \quad (3.58)$$

The exponent that scales order-parameter is called β

$$m \sim \varepsilon^\beta \quad (3.59)$$

Another exponent that scales order-parameter is called δ , but it relates the order parameter with the magnetic field, h

$$m \sim h^\delta \quad (3.60)$$

The exponent that scales susceptibility is called γ

$$\chi \sim \varepsilon^{-\gamma} \quad (3.61)$$

Note that these quantities only follows power law near T_c .

3.4.2 Rushbrooke Inequality

$$\alpha + 2\beta + \gamma \geq 2 \quad (3.62)$$

but the equality is often obtain theoretically which is shown below in the present case

$$\begin{aligned} \alpha + 2\beta + \gamma &= \frac{2a_\varepsilon - 1}{a_\varepsilon} + \frac{2(1 - a_h)}{a_\varepsilon} + \frac{2a_h - 1}{a_\varepsilon} \\ &= \frac{2a_\varepsilon}{a_\varepsilon} \\ &= 2 \end{aligned}$$

Thus the Rushbrooke inequality is satisfied.

3.4.3 Griffiths Inequality

$$\alpha + \beta(1 + \delta) = 2 \quad (3.63)$$

Let's do a quick check to see if this is also satisfied.

$$\begin{aligned} \alpha + \beta(1 + \delta) &= \frac{2a_\varepsilon - 1}{a_\varepsilon} + \frac{1 - a_h}{a_\varepsilon} \left(1 + \frac{a_h}{1 - a_h} \right) \\ &= \frac{2a_\varepsilon - 1}{a_\varepsilon} + \frac{1}{a_\varepsilon} \\ &= \frac{2a_\varepsilon}{a_\varepsilon} \\ &= 2 \end{aligned} \quad (3.64)$$

So the Griffiths Inequality is also satisfied.

3.5 Ising Model

For a very long time scientists have been trying to understand phase transition in different aspects. And for this purpose many different models have been provided for decades. The first model was provided by physicist Ernst Ising as a mathematical model of ferromagnetism in statistical mechanics. The Ising model was invented by the physicist Wilhelm Lenz (1920),

who gave it as a problem to his student Ernst Ising. The one-dimensional Ising model has no phase transition and was solved by Ising (1925) himself in his 1924 thesis [72]. But he provided a model in 1 dimension and proved that in 1 dimension phase transition is not possible and concluded that it is not possible in higher dimension as well. But it was proved later that in dimension $d \geq 2$ phase transition is possible [134, 92] which proved Ising wrong about his conclusion but he certainly gave a good insight for phase transition and hence the naming.

Consider a set Λ of lattice sites, each with a set of adjacent sites forming a d-dimensional lattice. For each lattice site $k \in \Lambda$ there is a discrete variable σ_k such that $\sigma_k \in \{+1, -1\}$, representing the site's spin. A spin configuration $\sigma = (\sigma_k)_{k \in \Lambda}$ is an assignment of spin value to each lattice site.

For any two adjacent sites $i, j \in \Lambda$ there is an interaction J_{ij} . Also a site $j \in \Lambda$ has an external magnetic field h_j interacting with it. The energy of a configuration σ is given by the Hamiltonian

$$H(\sigma) = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - \mu \sum_j h_j \sigma_j \quad (3.65)$$

Where the first sum is over pairs of adjacent spins counting every pair only once. And we use $\langle ij \rangle$ to indicate that i and j are nearest neighbors. μ indicates the magnetic moment. The negative sign on the second term is there by convention [13]. The configuration probability is given by the Boltzmann distribution with inverse temperature $\beta \geq 0$

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta} \quad (3.66)$$

where $\beta = (k_B T)^{-1}$ and the normalization constant

$$Z_\beta = \sum_\sigma e^{-\beta H(\sigma)} \quad (3.67)$$

is the partition function. For a function f of the spins, which is the observable here, we denote

$$\langle f \rangle_\beta = \sum_\sigma f(\sigma) P_\beta(\sigma) \quad (3.68)$$

the expectation value of f . The configuration probabilities $P_\beta(\sigma)$ represent the probability that the system is in a state with configuration σ in equilibrium.

The minus sign on each term of the Hamiltonian function $H(\sigma)$ is conventional. Using this sign convention, the Ising models can be classified according to the sign of the interaction: if, for all pairs i, j

$$J_{ij} \begin{cases} > 0, \text{ ferromagnetic interaction} \\ < 0, \text{ anti-ferromagnetic interaction} \\ = 0, \text{ non-interacting spins} \end{cases} \quad (3.69)$$

otherwise the system is called non-ferromagnetic.

In a ferromagnetic Ising model, spins tend to be aligned, meaning, the configurations in which adjacent spins are of the same sign have higher probability. In an anti-ferromagnetic model, adjacent spins tend to have opposite signs.

The sign convention of $H(\sigma)$ also explains how a spin site j interacts with the external field. Namely, the spin site wants to line up with the external field.

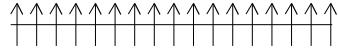
$$h_j \begin{cases} > 0, \text{ the spin site } j \text{ desires to line up in the positive direction} \\ < 0, \text{ the spin site } j \text{ desires to line up in the negative direction} \\ = 0, \text{ no external influence on the spin site} \end{cases} \quad (3.70)$$

Ising models are often examined without an external field interacting with the lattice, that is, $h = 0$ for all j in the lattice Λ . Using this simplification, our Hamiltonian becomes:

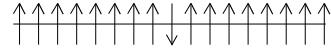
$$H(\sigma) = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \quad (3.71)$$

When the external field is everywhere zero, $h = 0$, the Ising model is symmetric under switching the value of the spin in all the lattice sites; a non zero field breaks this symmetry.

Another common simplification is to assume that all of the nearest neighbors $\langle ij \rangle$ have the same interaction strength. Then we can set $J_{ij} = J$ for all pairs i, j . In this case our Hamiltonian is further simplified to:



(a) all are in spin up state



(b) only one site is in spin down state

Fig. 3.9 One dimensional Ising model

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \quad (3.72)$$

Ising himself had provided the theory of his model for 1 dimensional case. He did not find any phase transition and concluded that phase transition is not possible in any dimension.

Consider an one dimensional lattice where all sites are in spin up state. Then according to Ising model their total energy E and entropy S is as follows

$$E = -N J \quad (3.73)$$

$$S = 0 \quad (3.74)$$

Where N is the number of sites on the lattice. Now if one of the sites is fliped then

$$E = -(N - 2)J \quad (3.75)$$

$$S = \log N \quad (3.76)$$

Therefore the cost is $\Delta E = 2J$ and change in entropy is $\Delta S = \log N$ for flipping spin of one site. The figure (3.9) shows this.

Therefore the change in free energy due to flipping one spin is,

$$\Delta F = \Delta E - T \Delta S \quad (3.77)$$

$$= 2J - T \log N \quad (3.78)$$

In the thermodynamic limit $N \rightarrow \infty$ the second term always dominates except for $T = 0$. Thus in one dimensional lattice there is phase transition at non zero temperature since we cannot have $\Delta F = 0$ (the transition point).

Now interesting this happens in case of two dimensional lattice. Say we have a square lattice of size N where there is an island of $L = 3$ sites of different spins (3.10).

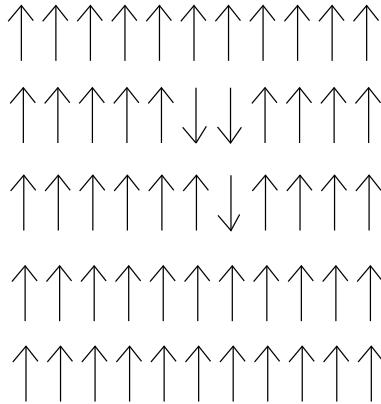


Fig. 3.10 Two dimensional Ising model with an island of 3 site with opposite spin state

$$\Delta E = 2LJ \quad (3.79)$$

$$\Omega = 3^L N \quad (3.80)$$

$$S = K \log \Omega \quad (3.81)$$

$$\Delta S = S - 0 = S \quad (3.82)$$

Therefore the free energy is

$$\Delta F = \Delta E - T \Delta S \quad (3.83)$$

$$= 2JL - KT \log(3^L N) \quad (3.84)$$

$$= 2JL - TL \log 3 - KT \log N \quad (3.85)$$

since at transition point $\Delta F = 0$ we get

$$0 = L(2J - T_c \log 3) \quad (3.86)$$

$$T_c = \frac{2J}{\log 3} \quad (3.87)$$

clearly $J \neq 0$ then $T_c \neq 0$. The exact solution is

$$T_c = \frac{2J}{\log(1 + \sqrt{2})} \quad (3.88)$$

Thus we can see that spontaneous magnetization (phase transition) is possible in 2D for a non zero T . And any higher dimensional lattice undergoes a transition for a non zero temperature.

Chapter 4

Percolation Theory

Percolation has been studied extensively in statistical physics due to the simplicity of its definition and the versatility of its application in seemingly disparate complex systems [113]. New models and variants of existing model is always welcome due to its importance and of wide interdisciplinary interests. In recent decades there has been a surge of research activities in studying percolation thanks to the emergence of network which has been used as the skeleton for percolation which can mimic structure of many natural and man-made systems.

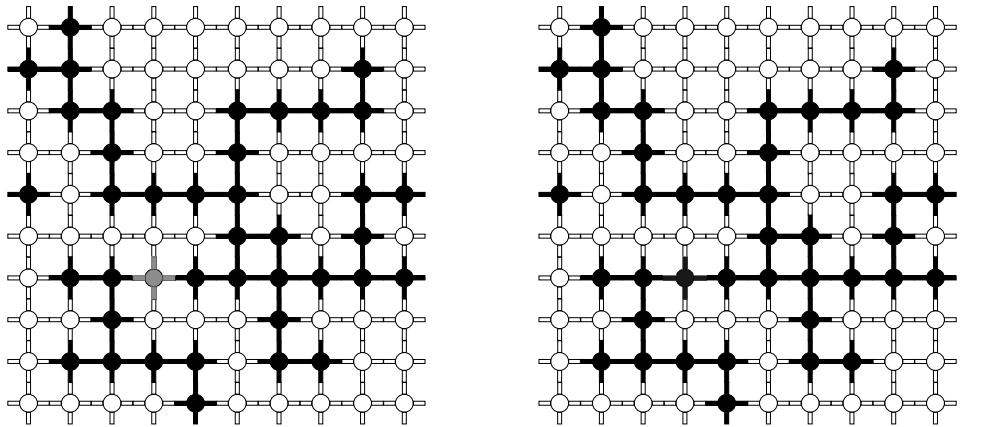
There are several reason to study percolation. First, it is easy to formulate and simple to implement as there is only one control parameter, called occupation probability p (4.4.1). The reason for its simplicity is that it requires neither quantum nor many particle interaction effects and yet it can describe phase transition and critical phenomena [112, 125]. Second, scientists use it as a theoretical model for phase transition, just like architects use geometric model before building large expensive structure, because of its simplicity. Third, it is well endowed with beautiful features and conjectures like finite-size scaling, universality just like its thermal counterpart. Fourth, besides being the paradigmatic model for phase transition, it has been found that the notion of percolation is omnipresent in a wide range of many seemingly disparate systems (4.9).

To study percolation theoretically, the first thing that one need is to choose a skeleton or playground, namely an empty lattice (or a graph/network), consisting of sites (or nodes) and bonds (or links). The definition of the percolation model is then so simple that it merely needs

a sentence to define it. Each site or bond of the chosen skeleton, depending on whether we want to study site or bond type percolation, is either occupied with probability p or remains empty with probability $1 - p$ independent of the state of its neighbors. Recently, percolation has received a renewed attention due to widening scope for using complex networks as a skeleton and due to widening extent of using various variants as a rule. In percolation most observable quantities this way or another is connected to clusters, group of contiguous occupied sites form a cluster, or to their distribution function. As the occupation probability p is tuned starting from $p = 0$, one finds that at certain value of $p = p_c$ the observable quantities undergoes a sudden and sharp change which is always regarded as a sign of phase transition. Indeed, the value at which such change occurs is called threshold or critical value which is equivalent to critical temperature of its thermal counterpart. The phase transition that percolation describes is purely geometrical in nature. It requires no consideration of quantum and many particle interaction effects and hence we can use it as a model for thermal Continuous Phase Transition (CPT) like architect use model before constructing large and complicated structure

4.1 Percolation Phenomena

The word 'Percolation' comes from the coffee percolator but it has nothing to do with coffee brewing. The only connection might be in the concept that lies behind the name. Let's start explaining the phenomena by example. Let's consider a square grid made of conductor of size $L \times L$ containing L^2 sites (insulator). Now we set up an arrangement to put a potential difference across the square grid and measure the effective resistance of the grid as well as the current. Suppose now we start taking of the sites one by one at a random and place a conductor there. We define a parameter called Occupation Probability, p , which is the fraction of the sites replaced as conductor to the total number of sites. We visit all the sites and generate a random number and only if $r \leq p$ we replace the site with a conductor. We observe that the electric conductance of the grid will be found to increase with increasing sites being replaced by conductors. As the sites are being turned into insulators, the value of p changes. We see that at a certain value of p , the electricity starting flowing. This particular value is known as Percolation Threshold, p_c . This vanishing resistance occurs



(a) One step away to flow current from top to bottom only if the grey site is next to be occupied.
(b) Current flows from top to bottom for the first time, i.e. $p = p_c$.

Fig. 4.1 percolation phenomena in square structure. No current if $p < p_c$.

when a particular amount of sites turns into conductors from insulators that causes the system to get the connection between the two end across polarity. The exact value of p_c has been found to be close to 0.5927. One can never expect to get the value each time they perform this experiment, infact, the chance of getting this exact value at any experiment can be one in a million. So we do this same experiment a number of times and then average over the value to get a better result. This example shows a simple way of understanding the phenomenon that we call percolation. The theory which simulates this kind of phenomenon is known as Percolation Theory. It provides a quantitative description of the nature of continuous pathways through space. The usual objective of research implementing this phenomenon is to characterize some aspect of the critical phenomena of the phase transition between finite and infinite range connectivity. This is actually non-trivial when the space is randomly disordered and the connected regions acquire fractal properties [138, 88].

4.2 Historical Overview

In 1941, the idea of percolation was first conceived by Flory [53] in the context of gelation transition. But as a mathematical model, it was formulated in the late fifties, to understand the motion of gas molecules through the maze of pores in carbon granules filling a gas mask. This seminal work was done by Simon Broadbent and John Hammersley [27], an

engineer and a mathematician respectively. Later on, percolation problem was popularized in physics community by Cyril Domb, Michael Fisher, John Essam and M.F. Skyes [48, 51]. Another remarkable work was the observation of percolation to be the limiting case of the general Potts model, which includes the Ising model and can be solved exactly which is done by Fortuin and Kasteleyn in 1969 [75]. This work paved the way to many exact results in percolation, and also allowed the usage of powerful re-normalization group ideas [31]. Finding percolation threshold both exactly and by simulation has been an enduring subject of research in this field [116], as well as the development of algorithms such as those by Hoshen and Kopelman [67], by Leath [81], and by Newman and Ziff [98] (which we have used in our research). Finding rigorous proofs of exact thresholds and bounds has also been an enduring area of research for mathematicians (Kesten [76], Wierman [131], Bollobas and Riordan [24] etc.) Another infusion of interest in percolation came from the surging field of network theory which goes back to the study of random and complete graphs by Erdos-Renyi(1959). In ER model, an observation of made of formation of a giant component, this giant component is exactly analogous to the formation pattern in percolation [45, 46]. It was then revitalized by interest in the small world phenomenon and Scale free networks. In 2000, Newman and Moore found the critical point for a random graph in the limit of large size, in which case the system is effectively a Bethe lattice, and this result connects to the early work of Flory, Fisher and Essam, but it was found with a general degree distribution [93]. In the field of random networks, the model of explosive percolation was first introduced by Achlioptas, D’Souza and Spencer [8], and this has been another fascinating problem which has led to a wave of new interest in percolation.

4.3 Classifications and Playground

Any percolation problem have two major parts, one is the rule which states how and what to occupy and connect and another is a playground on which we apply the rules. The term spanning cluster is the cluster that connects the opposite boundary of a playground. If, however, the system has no boundary then it is measured in terms of largest cluster and is called Giant Connected Component or GCC and it only appears if the system has reached or passed the threshold.

4.3.1 Types of Percolation

Since the first percolation model studied was Bernoulli percolation (In this model all bonds are independent. This model is called bond percolation by physicists) through time physicists have defined different types of percolation model in different types of skeleton or playground. Here we discuss some of the most used percolation types.

Bond Percolation

In bond (or edge, link) percolation we occupy the bonds with probability p and we use sites to connect the bonds together. The cluster size is measured in terms of the number of sites in the cluster. If p is below a critical value p_c then there is no spanning cluster (or GCC) and if $p \geq p_c$ then we will have a spanning cluster or GCC.

Site Percolation

In site (or vertex, node) percolation we occupy the sites. According to the definition of site percolation we use sites to measure the cluster size. But in order to keep it consistent with the laws of thermodynamics we have changed the definition [108]. Now we use bonds to measure the cluster size while we occupy sites. This change of definition does not effect the exponent that describe the phase transition. Before the critical point where $p < p_c$ there is not spanning cluster and if $p = p_c$ the spanning cluster appears for the first time and it remains as the largest cluster of the system. All the property that describes the phase transition are present at $p = p_c$ and this is where we study them.

Explosive Percolation

In 2009 Achlioptas et al. proposed a biased occupation rule, known as the Achlioptas process (AP), that encourages slower growth of the larger clusters and faster growth of the smaller clusters instead of random occupation in classical percolation [8]. According to this rule a pair of links or, bonds are first picked uniformly at random from all possible distinct links. However, of the two, only the one that satisfies the pre-selected rule is finally chosen to occupy and the other one is discarded. The preset rule is usually chosen so that it discourages the growth of the larger clusters and encourages the growth of the smaller clusters. As a result,

the percolation threshold is delayed and hence the corresponding p_c is always higher than the case where only one bond is always selected. Furthermore, it is natural to expect that close to p_c nearly equal sized clusters, waiting to merge, are so great in number that occupation of a few bonds results in an abrupt global connection and thus the name "Explosive Percolation" (EP). Investigation of Achlioptas processes on different types of substrate networks and with different choices of rules especially with the aim of developing rules that do not use global information about a graph is an active area of research.

K-Core Percolation

The K -core of an unweighted, undirected network is the maximal subset of nodes such that each node is connected to at least K other nodes [119]. Determining K -cores computationally is fast and they are insightful in many situations [43, 40]. Every undirected, unweighted network has a K -core decomposition. K -shell of a network is defined as the set of all nodes that belong to the K -core but not to the $(K + 1)$ - core. K -core is given by the union of all c -shells for $c \geq K$ and the K -core decomposition is the set of all of its c -shells. One can examine the K -core of a network as the limit of a dynamical pruning process. Starting with the initial network we delete all nodes with fewer than k neighbors. After this pruning, the degree of some of the remaining nodes will have been reduced. Repeating this process to delete nodes will give a network which will have fewer than K remaining neighbors. Iterating this process until no further pruning is possible leaves the K -core of the network [106].

Bootstrap Percolation

Bootstrap percolation is an infection-like process in which nodes becomes infected if sufficiently many of their neighbors are infected [9]. In bootstrap percolation, sites on an empty lattice are first randomly occupied and then all occupied sites with less than a given number m of the occupied neighbors are successively removed until a stable configuration reached. On any lattice for sufficiently large m , the ensuing clusters can only be infinite. On a Bethe lattice for $m \geq 3$, the fraction of the lattice occupied by infinite clusters discontinuously jumps from zero at the percolation threshold. From an analysis of stable and metastable ground state of the dilute Blume-Capel model [20], it is concluded that the effects like bootstrap percolation may occur in some real magnets [33].

Other

Apart from the type of percolation process described briefly above there are numerous other types of percolation. In *Limited Path Percolation*, one construes "connectivity" as implying that sufficiently short path still exists after some network components have been removed [83]. The percolation of K -cliques (completely connected sub-graphs of K nodes) has been used to study the algorithmic detection of dense sets of nodes known as "communities" [102]. Various percolation processes have also been studied in several different types of multi-layer networks (e.g. multiplex networks and interdependent networks) [22, 78]. Another class of models results if we remove the restriction of a lattice and allow particles to occupy positions which vary continuously in space. *Continuum Percolation* [60, 104, 23], as it is called, suffers from the added complication that tricks which can sometimes be used on lattice models cannot be applied. A quite different process as *Invasion Percolation* [58, 86, 133]; its invention was prompted by attempts to understand flow in porous media. Random numbers are assigned to each site of a lattice. Choose a site, or sites, on one side of the lattice and draw a bond to the neighbor which has the lower random number assigned to it. (The growing cluster represents the invading fluid with the remainder of the sites representing the initial, or defending, fluid). This process continues until the cluster reaches the other side [82].

4.3.2 Types of Playground

Apart from the rules we need a playground to study percolation. Most used playground is described in the following.

Lattice

Percolation was mainly studied on different types of lattice. For example, Honeycomb lattice, Bethe lattice, Simple Cubic lattice, Body-Centered-Cubic lattice, Face-Centered-Cubic lattice. In 1998 Christian D. Lorenz et al. did extensive Monte Carlo simulation to study bond percolation on the simple cubic, face-centered-cubic and body-centered-cubic lattices using epidemic approach. There simulations provide very precise values of the critical thresholds [84]. They calculated Fisher exponent, τ , the finite-size correction exponent, Ω and the scaling function exponent, σ confirmed to be universal. They also did percolation on

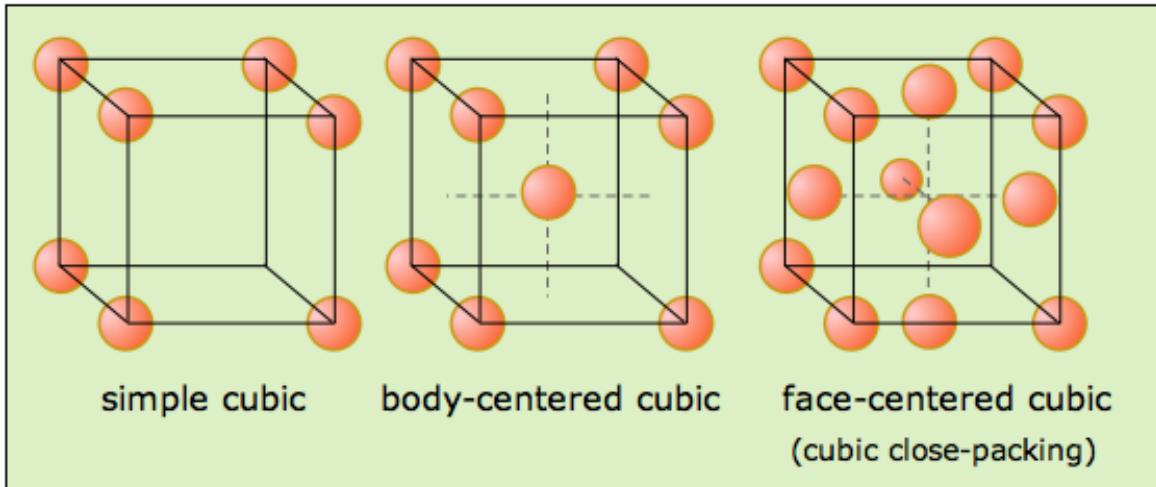


Fig. 4.2 Different types of cubic lattice [1]

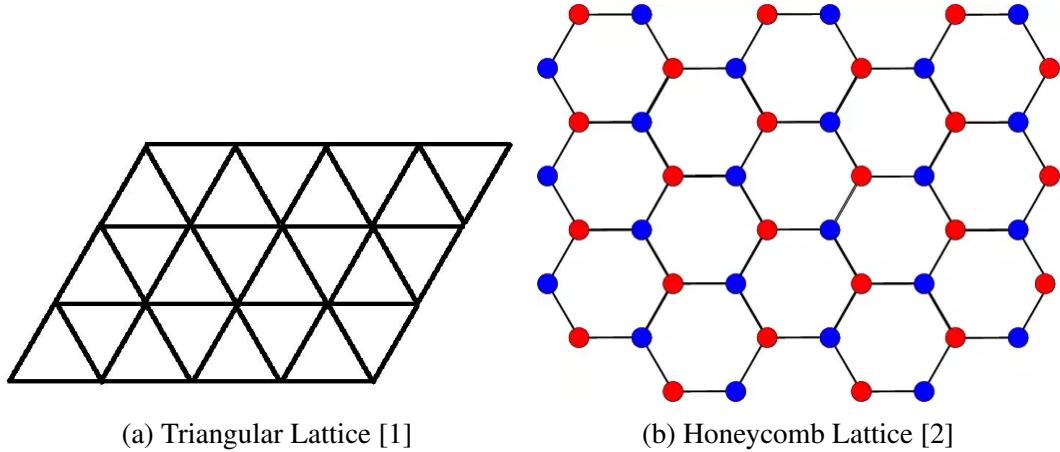


Fig. 4.3 Different types of cubic lattice

the HCP (hexagonal closed packed) lattice [85]. Before that in 1981 JC Wireman studied bond percolation on honeycomb and triangular lattices [132].

Furthermore, an exact solution on Bethe lattice for high density percolation was done by G. R. Reich and P. L. Leath in 1978 [109] and J. Chalupa et al. did bootstrap percolation on Bethe lattice in the following year [33].

Graph or Network

A new playground was added to the world of percolation in 1959 when two prominent mathematicians of all time, Paul Erdos and Alfred Renyi introduced Random Graphs [1]. Before

that, it was mostly popular among the mathematicians but not that much fascinating for most of the physicists because of its abstraction. But with the advent of scale free networks [7] which mimics the real life networks such as citation network, social network, protein-protein interaction, in 1999, physicists became much more interested in random networks. The difference in the terminology like graphs and networks are just graphs are mostly used by mathematicians and computer scientists and networks is mainly referred by physicists to the same concept. Duncan S. Callaway and his group did percolation study to find robustness and fragility [29]. Clique percolation is also studied on random networks [42]. A critical phenomenon analysis on random networks for core percolation is done by Bauer [16]. In early 80's, before the birth of scale free networks, C McDiarmid did two significant works which you can find in the references [1].

Reuvan Cohen et al. studied scale free networks close to the percolation threshold [37]. N. Schwartz et al. worked on percolation problem in directed scale free networks [117]. Filippo Radicchi and Santo Fortunato studied scale-free networks constructed via a cooperative Achlioptas Growth Process [8]. They showed that networks constructed via this biased procedure show a percolation transition which strongly differes from the one observed in standard percolation, where links were introduced just randomly.

4.4 Basic Elements

In this section we discuss some of the basic elements of percolation. All the observable quantities depends on these elements.

4.4.1 Occupation Probability

The probability at which each site (bond) is occupied is called occupation probability in site (bond) percolation and it is denoted as p . In section (4.8) we discuss who we determine p in percolation. Simply saying, instead of fixing p for one experiment we can find all quantity for each values of p using the famous Ziff algorithm [97, 98].

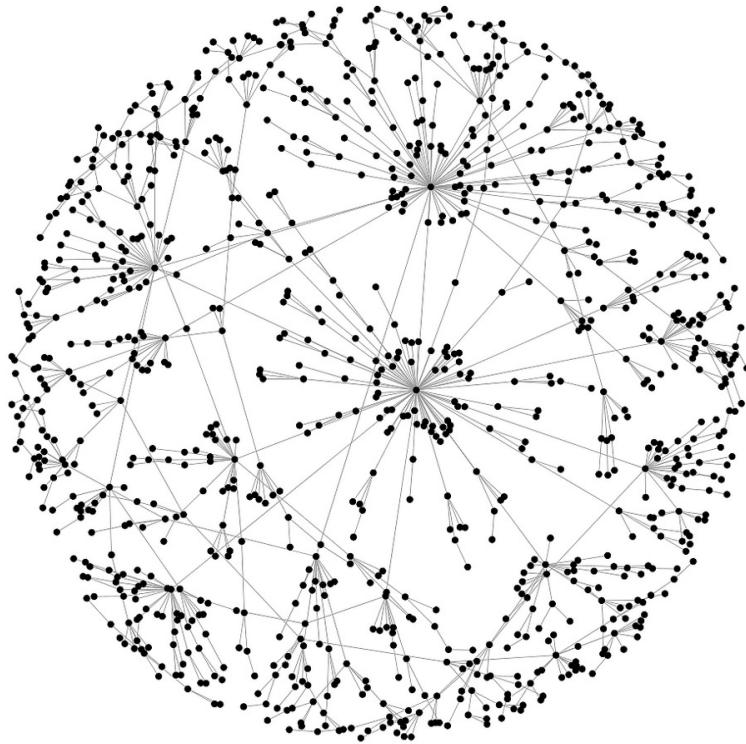


Fig. 4.4 Scale Free Network [3]

4.4.2 Cluster

Cluster is a collection of sites and bonds. In bond percolation we occupy bond and measure cluster size in terms of the number of sites in it. And following this idea we measure the cluster size in terms of the number of bonds in it. Which is the new definition of site percolation [108]. Measuring cluster size in terms of the number of bonds in it in site percolation reproduces all known results and it is consistent with laws of thermodynamics.

4.4.3 Spanning cluster

When occupying sites one by one randomly, we reach in a state where there emerges a special type of cluster. This cluster spans the entire lattice top to bottom or left to right for non periodic case. And for periodic case this cluster wraps around the lattice. This is the largest cluster on the lattice and it is absent before p_c and always present after p_c . This cluster is called the spanning cluster. And p_c is called the critical occupation probability.

4.5 Finite Size Scaling

We discussed Finite Size Scaling hypothesis in section (2.4.2) and commented that it is very useful in percolation theory. Here we will be making use of the FSS hypothesis for using in our work.

The correlation length is finite and defined as

$$\xi \sim (p - p_c)^{-\nu} \quad (4.1)$$

At $p \rightarrow p_c$, the lattice size $L \sim \xi$ we get

$$L \sim (p - p_c)^{-\nu} \quad (4.2)$$

In terms of $p - p_c$

$$(p - p_c) \sim L^{-1/\nu} \quad (4.3)$$

Now if we have a quantity that diverges at the threshold (critical point), then we can write the quantity say X to follow a power law

$$X \sim (p - p_c)^{-a} \quad (4.4)$$

Using (4.3) we get

$$X \sim L^{a/\nu} \quad (4.5)$$

We notice that X and $(p - p_c)$ both depends on L . At this point we introduce the Buckingham π theorem (2.2) and define two dimensionless parameter as

$$\Pi_1 = \frac{(p - p_c)}{L^{-1/\nu}} \quad (4.6)$$

$$\Pi = \frac{X}{L^{a/\nu}} \quad (4.7)$$

Now according to the definition of the dimensionless quantity, the numerical value of Π remains invariant even after the value of L is changed arbitrarily. So we can write

$$\Pi = \Phi(\Pi_1) \quad (4.8)$$

$$\frac{X}{L^{a/v}} = \Phi\left(\frac{p - p_c}{L^{-1/v}}\right) \quad (4.9)$$

$$X = L^{a/v} \Phi_X\left((p - p_c)L^{1/v}\right) \quad (4.10)$$

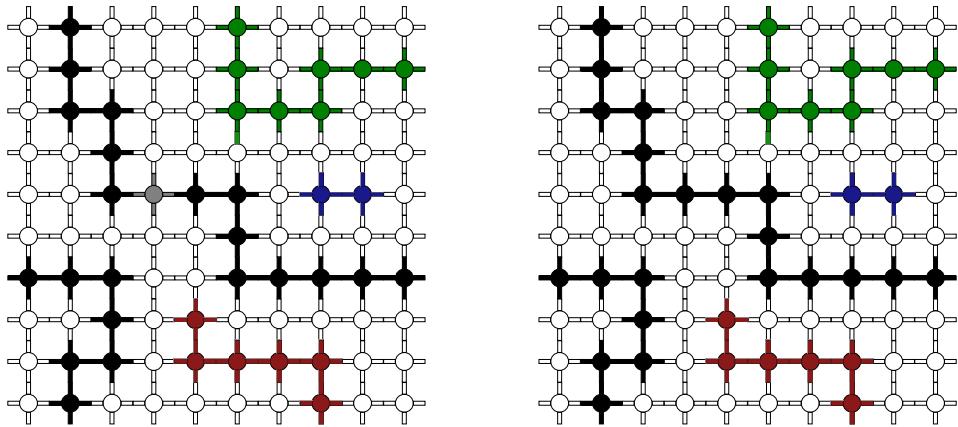
We note that by studying FSS hypothesis and applying it to find a relation between a quantity X as a function of finite system size or lattice length L at $p \rightarrow p_c$, we are able to find the exponent a/v .

4.6 Observable Quantities

In percolation we study formation of clusters, their properties such as how they are distributed as a function of control parameter p . A cluster is a group of occupied bonds (sites) in site (bond) percolation [108]. With no gap or unoccupied object between them. In a network cluster is defined as a group of nodes that connects the links. In this section we discuss some of the most used observable quantities in percolation.

4.6.1 Percolation Threshold, p_c

The idea of percolation threshold is a mathematical concept that deals with formation of long range connectivity in random systems. While there are no existence of a giant connected component that are talked about below the threshold, its existence is well present above it. As the occupation probability increases from 0 toward 1, average cluster size also increases and among all cluster one cluster pops up to be the spanning cluster at p_c . Hence p_c is the percolation threshold or critical point. In the thermodynamic limit this cluster becomes infinitely large. Thus for $p < p_c$ there is no spanning cluster and for $p \geq p_c$ there is one. The spanning cluster is a special type of cluster which spans the entire lattice. In periodic case we call it wrapping cluster. A figure illustrating this process is given here (4.5). Percolation



(a) One step away from threshold. Since the grey site is not occupied. The moment it gets occupied we reach percolation threshold

(b) The grey site gets occupied and a wrapping cluster appears for the first time. We have reached percolation threshold

Fig. 4.5 A square lattice of length $L = 10$. Demonstrating the appearance of the wrapping cluster

threshold has been determined for different types of lattices. The table (4.1) shows some of them.

Lattice	p_c , site percolation	p_c , bond percolation
Body Centered	0.246	0.1803
Face Centered	0.198	0.119
Simple Cubic	0.3116	0.2488
Diamond	0.43	0.388
Honeycomb	0.6962	0.65271
Triangular	0.50	0.34729
Square	0.592746	0.50

Table 4.1 Percolation Threshold for Some Regular Lattices

One simple way of obtaining p_c is to perform M number of independent experiment for a particular L and then take the average

$$p_{c_{avg}} = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_i p_{c_i} \quad (4.11)$$

But performing infinite number of experiment is not possible. So we use another approach which is described in section (4.6.2) and (5.2.1)

4.6.2 Spanning Probability, $w(p, L)$

The best quantity for finding the critical exponent v is the spanning probability $W(p, L)$. It describes the likelihood of finding a cluster that spans across the entire system of length L either horizontally or vertically at a given occupation probability p . To find $W(p, L)$ we perform say M independent realizations under the same identical conditions. In each realization for a given finite system size we take record of the p_c value at which there appears a spanning cluster for the first time. If there is a spanning cluster at $p = p_{c_i}$ then it means that there exists a spanning cluster for all $p_{c_i} \leq p \leq 1$. To find a regularity or a pattern among all the M numbers of p_c values recorded, one usually looks at the relative frequency of occurrence within a class or width Δp . To find $W(p, L)$, we can process the data containing M number of p_c values to plot histogram displaying normalized relative frequency as a function of class of width Δp chosen as per convenience [108]. Figure (5.10) shows spanning probability $w(p, L)$ as a function of p and L . Clearly all curves meet at a specific point regardless of system length L . Thus we can say if $L \rightarrow \infty$ the curve would still go through that point and that's how we get the p_c value. Then if we apply scaling on the x -axis by $(p - p_c)L^{1/v}$ we would get a perfect data collapse for a specific $1/nu$ that is our exponent. This process is discussed further in section (5.2.1) and (5.2.2).

4.6.3 Entropy, $H(p, L)$

Entropy is one of the key features of a phase transition model. But thermodynamic entropy, e.g. Boltzmann entropy or Clausius entropy, cannot be calculated for any model that depends on a probabilistic theory such as our percolation on a square lattice model. So we take our approach in another way. Information entropy or the *Shanon entropy* is best suited for our model. The concept of Shannon entropy in information theory describes how much information there is in a signal or event. This concept of information entropy was introduced by Claude Shannon in his 1948 [121]. The seminal work of Shannon based on papers by Nyquist [99, 100] and Hartley [62]. He rationalized these early efforts into a coherent mathematical theory of communication.

The Definition of Shannon entropy is

$$H = - \sum_i \mu_i \log \mu_i \quad (4.12)$$

where, μ_i is the probability of getting i -th element.

As we have seen in section (3.2.1) that the entropy measures disorderliness of a system. It is also easy to understand order and disorder in solid to liquid transition. But it is not that easy in percolation since the idea of order and disorder in percolation is not yet clear. To understand disorder, let us consider that at $p = 0$ we have 12 isolated sites and each has different color to identify them visually, figure (4.6). Thus each color corresponds to one distinct cluster. Occupation of a bond means merging of two colors into one. If one of the components is bigger in size than the other then the newly merged cluster will take the color of the bigger cluster and if they are equal then we choose one at random. If we now continue to occupy all the frozen bonds then we will finally have one cluster of one color. Initially at $p = 0$ we have 12 different colors and hence it can easily be regarded as the most disordered state. On the other hand, at the other extreme we will have only one cluster represented by one color which can be regarded as the ordered state. We can easily extend the problem to a system that contains N number of sites but colored with 12 colors only such that n_1, n_2, \dots, n_{12} of them are red, orange, ..., violet respectively and hence we can define $\mu_i = n_i/N$. We now make M number of independent attempts to pick one site at each attempt from N sites at random with uniform probability. Say, that we found n'_1 times red, n'_2 times orange, and so on such that $\sum_{i=1}^m n'_i = M$. We assume that both N and M are sufficiently large and $M \approx N$. The total number of ways we could have M outcomes are

$$\Omega = \frac{M!}{(M_{\mu_1})! (M_{\mu_2})! \dots (M_{\mu_m})!} \quad (4.13)$$

since $n'_i \approx M_{\mu_i}$. Taking log on both side of the above equation and using the String's approximation $\log(M!) = M \log M - M$ for very large M we get

$$\begin{aligned}
 \log \Omega &= \log M! - \log \left(\prod_i M_{\mu_i} \right) \\
 &= M \log M - M - \sum_i \log(M_{\mu_i}!) \\
 &= M \log M - M - \sum_i [M_{\mu_i} \log M_{\mu_i} - M_{\mu_i}] \\
 &= M \log M - \sum_i M_{\mu_i} \log M_{\mu_i} \\
 &= M \log M - M \sum_i \frac{M_{\mu_i}}{M} \left[\log \left(\frac{M_{\mu_i}}{M} \right) + \log M \right] \\
 &= M \log M - M \sum_i \mu_i \log \mu_i + M \sum_i \frac{M_{\mu_i}}{M} \log M
 \end{aligned} \tag{4.14}$$

Finally we have,

$$\log \Omega = -M \sum_{i=1}^m \mu_i \log \mu_i = MH(\mu) \tag{4.15}$$

where $H(\mu)$ is nothing but the Shannon entropy $H(p)$ and clearly it is the degree of uncertainty per attempt. Total entropy or information is therefore equal to NH if we consider $M = N$. In the case when each site has distinct color then each site will have the equal chance of being picked. It means $\mu_i = 1/N \forall i$ and hence $H(\mu) = N \log(N)$ which is the average entropy or degree of disorder and the total entropy is $NH(\mu)$. Now initially if we had N distinct color then the system would have the maximum entropy $S = N \log N$. On the other hand, if all the sites had the same color then the system would have minimum entropy $S = 0$. Thus percolation is indeed an order-disorder transition where disorder is equivalent to degree of confusion [108]. Now recall the definition of Boltzmann entropy in equation (3.19). If we consider $K_B = 1$ then we get Shannon entropy to represent Boltzmann entropy.

worked out example

Say we have a coin with a head and a tail. If the coin is unbiased then the probability of getting the head or the tail is 50% or 0.5. Now what's the entropy of this system? The Shanon entropy is the one that can be used here. For convenience \log_2 will be used for

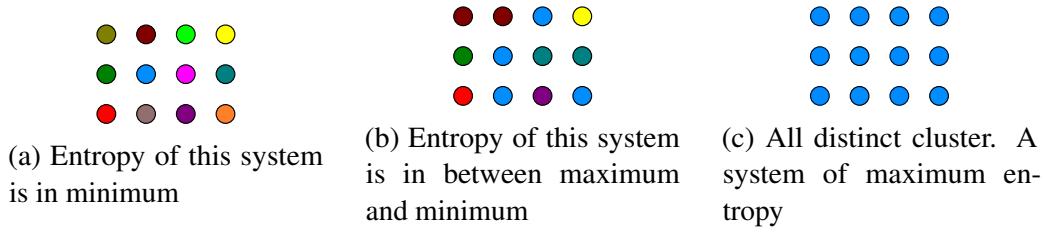


Fig. 4.6 A system of 12 cluster

evaluating logarithms here, after all $\log_2 = \text{const.} \log_{10} = \text{const.} \log_e$. Here, $\mu_i = 0.5$ and $\log_2(0.5) = -1$, Therefore we have

$$\begin{aligned} H &= -(0.5 \log_2(0.5) + 0.5 \log_2(0.5)) \\ &= -(0.5 \times (-1) + 0.5 \times (-1)) \\ &= 1 \end{aligned}$$

so in this system entropy is 1.

Now take a new system where there is 4 identical object. Since all objects are identical, each have probability $\mu_i = 1/4$ and $\log_2(1/4) = -2$. Then the total entropy of that system is 2. So this is clear that the entropy increases with the increase of the system size. Here system size is determined by the number of particles in it. Now, let's take a non-uniform system, where there are total 8 particles and there are 4 cluster. Cluster 1 has 4 particles and cluster 2 has 2 particles and other 2 cluster of 1 particle each. Probability of getting cluster 1 is $\mu_1 = 4/8$ and for cluster 2 it is $\mu_2 = 2/8$ and for other clusters it is $\mu_3 = \mu_4 = 1/8$. Now the entropy of the system becomes,

$$\begin{aligned} H &= -\sum_i \mu_i \log_2 \mu_i \\ &= -(4/8 \log_2(4/8) + 2/8 \log_2(2/8) + 1/8 \log_2(1/8) + 1/8 \log_2(1/8)) \\ &= -(-1/2 - 1/2 - 3/8 - 3/8) \\ &= 7/4 \end{aligned}$$

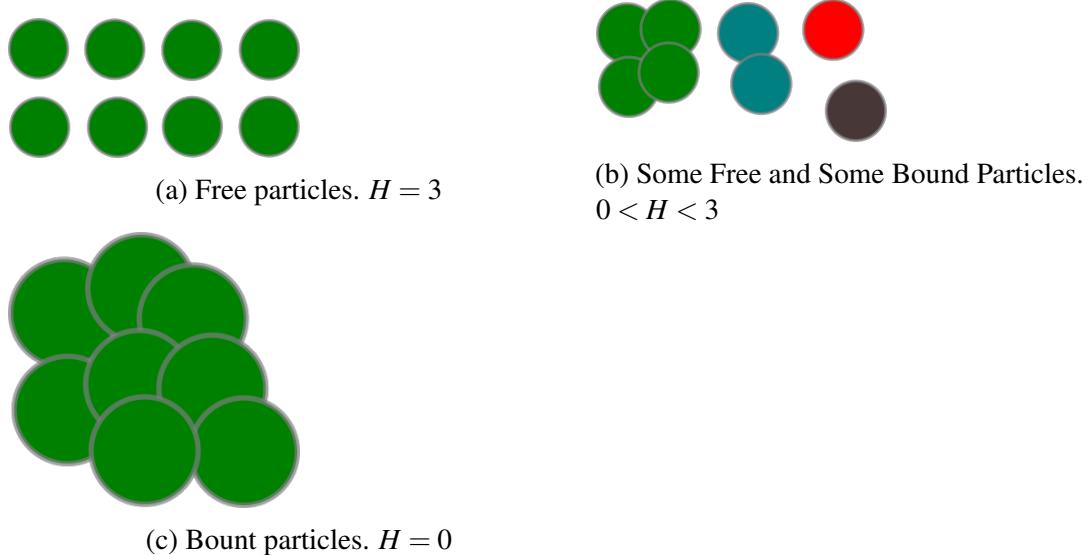


Fig. 4.7 entropy of a system of 8 particles

which is less than the entropy of a system where all 8 particles are disconnected, i.e., $H = 3$. So we can see that as the particles are joined together entropy reduces, which is in agreement with the experimental results.

4.6.4 Specific Heat, $C(p, L)$

According to the definition of specific heat in thermodynamics (3.27) we can find specific heat if we know the temperature and entropy. In percolation theory we measure the Shannon entropy, $H(p, L)$. And we use $(1 - p)$ as the analogue of temperature which gives

$$C = (1 - p) \frac{dH}{d(1 - p)} \quad (4.16)$$

$$= -(1 - p) \frac{dH}{dp} \quad (4.17)$$

using this definition we can easily find the specific heat of the percolating system. And from specific heat we obtain the critical exponent α from the scaling relation in section (3.4.1) which turns out to be

$$C = L^{\alpha/\nu} \phi_C((p - p_c)L^{1/\nu}) \quad (4.18)$$

Here we have used FSS hypothesis (4.5). Therefore plotting $CL^{-\alpha/\nu}$ vs $(p - p_c)L^{1/\nu}$ would give us a data collapse.

4.6.5 Order Parameter, $P(p,L)$

From above discussion we can say that if $p \geq p_c$ the spanning cluster exists but we still cannot say if a randomly chosen site belongs to the spanning cluster. Therefore we need to quantify the strength of the spanning cluster. Percolation strength or P is defined as the probability to find the site that belongs to the spanning cluster, meaning randomly pick a site and what is the probability that the selected site will belong to the spanning cluster. And this quantity should depend on occupation probability p and system size L . We call it Percolation Strength or sometimes Order Parameter as it describes the measure of order in the system. Order means the likeliness of not getting confused. If all clusters of same size, i.e. identical, we will get confused which cluster we have chosen ($p = 0$ case) but if there is only one cluster there is no chance of confusion ($p = 1$ case).

We define the percolation strength as

$$P = \frac{\text{number of sites in the spanning cluster}}{\text{total number of sites in the lattice}} \quad (4.19)$$

But in a system where there are no boundary, e.g. a network or Bethe lattice, the idea of spanning cluster is not valid. Then we use the largest cluster to define the percolation strength

$$P = \frac{\text{number of nodes in the largest cluster}}{\text{total number of nodes in the network}} \quad (4.20)$$

Both definition, though looks a bit different when plotted, gives the same critical exponent β . How to find this exponent is shown in section (5.2.4).

Mathematically

$$P(p,L) = \frac{K}{\sum_i k_i} \quad (4.21)$$

where K is the size of the spanning cluster and k_i is the size of the $i - th$ cluster. Percolation strength is the Order parameter of the system which is the measure of Order of a system.

Note that, with periodic boundary condition we have

$$\sum_i k_i = L^2 \quad (4.22)$$

and without periodic boundary condition

$$\sum_i k_i = L(L-1) \quad (4.23)$$

Order parameter is related to the exponent β from the scaling relation in section (3.4.1) which turns out to be

$$P = L^{-\beta/\nu} \phi_P((p - p_c)L^{1/\nu}) \quad (4.24)$$

Here we have used FSS hypothesis (4.5). Therefore plotting $PL^{\beta/\nu}$ vs $(p - p_c)L^{1/\nu}$ would give us a data collapse.

4.6.6 Susceptibility, $\chi(p, L)$

In percolation we measure susceptibility using jumps of the size of the largest cluster, i.e., ΔP . We keep track of the size of the largest cluster for each change of p , i.e. Δp . Then the jump per unit change of p tells us what the susceptibility is. Mathematically

$$\chi = \frac{\Delta P}{\Delta p} \quad (4.25)$$

for a lattice of length L there are L^2 sites and occupying one site increase p by $1/L^2$ therefore for site percolation $\Delta p = 1/L^2$ and for bond percolation it is $\Delta p = 1/2L^2$. Susceptibility can also be measured by differentiating the order parameter P with respect to p and it would give the same exponent upon measurement.

Susceptibility is related to the exponent γ from the scaling relation in section (3.4.1) which turns out to be

$$\chi = L^{\gamma/\nu} \phi_\chi((p - p_c)L^{1/\nu}) \quad (4.26)$$

Here we have used FSS hypothesis (4.5). Therefore plotting $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ would give us a data collapse.

4.6.7 Fractal Dimension, d_f

A fractal [49] is an object which occupies less space than it is embedded. For example a piece of cheese is a 3D fractal, since there are holes in the cheese which is empty. The spanning cluster shows a behaviour to be a fractal. The spanning cluster is a unique cluster that spans the entire lattice (or wraps around the lattice). But the size of the spanning cluster varies with the size of the lattice and it is related as

$$S \sim L^{-d_f} \quad (4.27)$$

here S is the size of the spanning cluster and d_f is known as the fractal dimension. If we plot $\log S$ vs $\log L$ we will find a straight line with negative slope which has value d_f . Thus d_f gives us the size of spanning cluster for a lattice of length L .

4.6.8 Cluster Size Distribution Function, n_s

At the critical point there exists many clusters of different sizes. Say we have m distinct cluster meaning none of the m clusters are of same size. n_1, n_2, \dots, n_m is the number of times cluster of size $1, 2, \dots, m$ appears divided by the total number of cluster. Therefore we will have

$$\sum_s n_s s = 1 \quad (4.28)$$

where s is the size of a cluster and n_s is the frequency of the occurrence of the cluster of size s . They seem to follow the power law

$$n_s(p_c) \sim s^{-\tau} \quad (4.29)$$

Thus if we know the size of the cluster at p_c we can tell approximately the number of time that cluster appears and vice versa.



Fig. 4.8 One Dimensional Lattice. Empty ones are white and filled ones are black.

4.7 Exact Solutions

Percolation problem can be solved exactly in 1 and ∞ dimension. In dimension $1 < d < \infty$ there is not analytical solution, it can only be solved approximately using simulations. Analytic solution in dimension greater than 1 and less than ∞ is still to be solved problem. Interestingly, many of the features found in one dimension seem to be valid for higher dimensions too. Thus using the insight of these exact solutions in 1 and ∞ dimension we get a window into the world of phase transitions, scaling and critical exponents.

4.7.1 One Dimension

Threshold

The simplest lattice one can think of is the one dimensional lattice. It consists of many sites arranged at an equidistant positions along a line. Each site of the lattice can either be occupied with probability p or remain empty with probability $1 - p$. Thus there are only two possible states of each site. A cluster is a group of neighboring occupied sites which contains no empty sites in between. A single empty sites splits a cluster into two clusters. If we find n successive occupied sites, we say that it forms a cluster of size n . We want to find the probability at which an infinite cluster appears for the first time, i.e., the critical occupation probability.

Let $\omega(p, L)$ is the probability that a linear chain of size L has percolating cluster at probability p . Note that, if two sites form one cluster, the probability that we find such cluster is p^2 . Similarly if we want a cluster containing L sites the probability is $\omega(p, L) = p^L$, means L successive sites are occupied independent of each other.

$$\lim_{L \rightarrow \infty} \omega(p, L) = \begin{cases} 0, & \forall p < 1 \\ 1 \text{ only if } p = 1 \end{cases} \quad (4.30)$$

For $p = 1$ all sites of the lattice are occupied and a percolating cluster spans from $-\infty$ to ∞ so that each and every site of the lattice belongs to the percolating cluster. For $p < 1$ we will have on the average $(1 - p)^L$ empty sites. So if $L \rightarrow \infty$, we have $(1 - p)^L \rightarrow \text{const.}$ revealing that there will be at least one, if not more, empty site somewhere in the chain. Which proves that as long as $p < 1$ there is no spanning cluster. Thus the percolation threshold or the critical occupation probability in one dimension is

$$p_c = 1 \quad (4.31)$$

Cluster Size

A cluster of size s , a.k.a. s -cluster, is formed when s successive sites are occupied and they are surrounded by two empty sites. Probability of s successive sites being occupied is p^s and 2 sites are unoccupied is $(1 - p)^2$. Thus the probability of picking a cluster at random that belongs to an s -cluster is

$$n_s = p^s(1 - p)^2 \quad (4.32)$$

n_s is also the number of s -clusters per lattice site. Note that the state of one particular site is independent of any other sites, that's why we multiply probabilities. Further manipulation of equation (4.32) gives

$$n_s = (1 - p)^2 \exp(s \ln p) = (1 - p)^2 \exp(-s/\xi) \quad (4.33)$$

where ξ is the correlation length and defined as

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln(p_c - (p_c - p))} \sim (p - p_c)^{-1} = (p - p_c)^\nu \quad (4.34)$$

in the limit $p \rightarrow p_c$ and since $p_c = 1$.

Mean Cluster Size

The probability that an arbitrary site is in s -cluster is larger by a factor of s . This site can be any of the sites in the s -cluster. The probability that an arbitrary chosen site belongs to a cluster of size s is $n_s s$, since n_s is known to be the number of s -clusters per lattice site. Every

occupied site must belong to one cluster even if it is a cluster of only one site, i.e., a cluster of size unity. The probability that an arbitrary site belongs to a cluster is therefore proportional to the probably p that it is occupied.

$$\sum_{s=1}^{\infty} sn_s = \frac{\text{number of total occupied sites}}{\text{number of total lattice sites}} = p \quad (4.35)$$

A quick check of the validity of equation (4.35) can be performed using equation (4.32).

$$\begin{aligned} \sum_{s=1}^{\infty} sn_s &= \sum_s s(1-p)^2 p^s \\ &= (1-p)^2 \sum_s sp^s \\ &= (1-p)^2 \sum_s p \frac{d(p^s)}{dp} \\ &= (1-p)^2 p \frac{d \sum_s p^s}{dp} \\ &= (1-p)^2 p \frac{dp(1-p)^{-1}}{dp} \\ &= (1-p)^2 p \left(\frac{1}{1-p} + \frac{p}{(1-p)^2} \right) \\ &= p \end{aligned} \quad (4.36)$$

Here we have used the series sum (4.37).

$$\begin{aligned} \sum_s p^s &= p + p^2 + p^3 + \dots \\ &= p(1 + p + p^2 + \dots) \\ &= p(1 - p)^{-1} \end{aligned} \quad (4.37)$$

An important question one can ask is that what is average size of the cluster that we are hitting. Since n_ss is the probability that an arbitrary site belongs to an s -cluster and $\sum_s n_ss$ is the probability that it belongs to any cluster. Thus we define w_s as

$$w_s = \frac{n_ss}{\sum_s n_ss} \quad (4.38)$$

w_s is the probability that the cluster to which an arbitrary occupied site belongs contain exactly s sites. The average cluster size S is therefore

$$S = \sum_s w_s s \quad (4.39)$$

This equation is very much similar to

$$\bar{x} = \int x p(x) dx \quad (4.40)$$

using equation (4.38) we get

$$\begin{aligned} S &= \frac{\sum_s n_s s^2}{\sum_s n_s s} \\ &= \sum_{s=1}^{\infty} \frac{s^2 n_s}{p} \\ &= \frac{(1-p)^2}{p} \sum_{s=1}^{\infty} s^2 p^s \\ &= \frac{(1-p)^2}{p} \left(p \frac{d}{dp} \right)^2 \left(\sum_{s=1}^{\infty} p^s \right) \\ &= \frac{(1-p)^2}{p} \left(p \frac{d}{dp} \right)^2 (p(1-p)^{-1}) \\ &= p(1-p)^2 \frac{d^2}{dp^2} (p(1-p)^{-1}) \\ &= p(1-p)^2 \frac{d}{dp} (1-p)^{-2} \\ &= p(1-p)^2 2(1-p)^{-3} \\ &= \frac{2p}{1-p} \\ &= \frac{1+p}{1-p} \end{aligned} \quad (4.41)$$

we can write

$$S(p) = \frac{1-p}{1+p} = \frac{p_c + p}{p_c - p} \quad (4.42)$$

using the fact that $p_c = 1$ in 1D lattice. This equation reveals that the mean cluster size diverges for $p \rightarrow p_c$ where the minus sign signifies that we are approaching from below p_c .

This is in sharp contrast with higher dimensional ones where we can approach to p_c from either end while in one dimension we cannot have access to the state $p > p_c$. We thus find the mean cluster size diverges following power law as we have [63]

$$S(p) \sim (p_c - p)^{-1} \quad (4.43)$$

We encounter the similar behaviour in the higher dimensions also.

Correlation Function and Correlation Length

The correlation function or pair connectivity $g(r)$ is the probability that a site at position r from an occupied site belongs to the same finite cluster. We are not including the contribution of the infinite cluster. This is valid infinite cluster does not exists as long as $p < 1$. Let $r = 0$ then $g(r = 0) = 1$ since the site at $r = 0$ is the selected occupied site by definition. For 1D case a site at r to be occupied and belongs to the same finite cluster, we will need r subsequent sites and the probability of getting this is p^r . Therefore

$$g(r) = p^r \quad (4.44)$$

It can also be expressed in terms of correlation length ξ

$$g(r) = \exp(\ln(p^r)) = \exp(-r/\xi) \quad (4.45)$$

where ξ is the correlation length (4.34).

Now that we have correlation function, we can define mean cluster size in terms of it

$$S = 1 + \sum_{r=1}^{\infty} g(r) \quad (4.46)$$

At this point it is evident that the cutoff cluster size s_ξ , mean cluster size $S(p)$, and correlation length ξ diverges at the percolation threshold. The divergence has the form of a simple power law of the distance from the critical occupation probability. In higher dimensional percolation problem this observation is also valid.

4.7.2 Infinite Dimension

Apart from one dimension percolation problem can be solved in infinite dimension. For this we need a suitable playground such as Bethe lattice. Bethe lattice lattice is a special type of lattice where each site has z neighbors and each branch gives rise to $(z - 1)$ other branches. Figure (4.9) shows the Bethe lattice for $z = 3$. Note that for $z = 2$ we have nothing but the one dimensional lattice.

Properties of infinite dimensional object

For a 3D object the surface area is has dimension to L^2 and volume as dimension L^3 . The same pattern is true of object in any dimension. If we denote area by A and volume by V for any dimension we have

$$A \propto V^{1-1/d} \quad (4.47)$$

now as $d \rightarrow \infty$ we have

$$A \propto V \quad (4.48)$$

Therefore if we find that the area of any object is proportional to its volume we can say it is an infinite dimensional object.

Bethe Lattice

In order to construct Bethe lattice for any z we start with a central point which will be connected to z sites. For example if $z = 3$ then we will have a central site connected to 3 sites by a branch and when we go to next layer each branch will be divided to 2 more branches and this process will be continued up to r layers (4.9). Only at the surface of the lattice, where the branching is stopped, is only one bond or branch connecting the surface site to the interior. There is only open loops in this structure, which means that if we never change direction always reach new site if we never go back. Number of sites in the Bethe lattice increases exponentially with the distance from the origin, whereas in any d -dimensional lattice structure it would increase with distance d . In the case of Bethe lattice with $z = 3$, the origin is surrounded by a shell of three sites ("first generation"), in the second shell we have six sites followed by a third generation of twelve sites, etc. After r generation the total

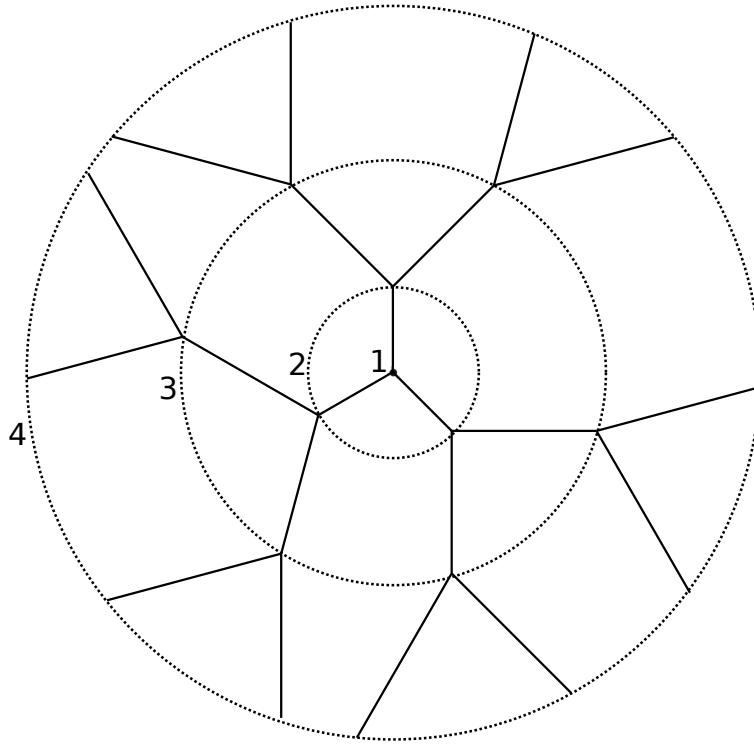


Fig. 4.9 Bethe Lattice for $z = 3$

number of sites in the Bethe lattice is

$$1 + 3 \times (1 + 2 + \dots + 2^{r-1}) = 3 \cdot 2^r - 2 \quad (4.49)$$

The number $3 \times 2^{r-1}$ is the number of sites at the surface. Here we have used the following finite series sum

$$1 + 2 + 2^2 + 2^3 + \dots + 2^r = 2^{r+1} - 1 \quad (4.50)$$

And if we measure the surface to volume ratio we get

$$\frac{A}{V} = \frac{\text{number of sites in the surface}}{\text{total number of sites}} = \frac{3 \times 2^{r-1}}{3 \times 2^r - 2} \quad (4.51)$$

as $r \rightarrow \infty$ we get

$$\frac{A}{V} \sim \frac{3 \times 2^{r-1}}{3 \times 2^r} = \frac{1}{2} = \text{constant} \quad (4.52)$$

Therefore Bethe lattice is indeed an infinite dimensional lattice.

Percolation Threshold

Percolation threshold of Bethe lattice is the occupation probability at which an infinite cluster appears for the first time. To find it we start walking from the origin and after one step we have $z - 1$ new bonds that is connected to $z - 1$ new sites in those direction. On the average there will be $(z - 1)p$ occupied sites. And for each site there will be another $z - 1$ branch and those bonds are connected to $(z - 1)p$ sites on the average and so on. After r step we will have an infinite cluster at probability $((z - 1)p)^r$. Since $r \rightarrow \infty$ we have $((z - 1)p)^r = 0$ if $(z - 1)p < 1$. Thus we choose $(z - 1)p = 1$ so that we will get an infinite cluster. That lead us to the desired critical occupation probability

$$(z - 1)p_c = 1$$

$$p_c = \frac{1}{z - 1} \quad (4.53)$$

For $z = 3$ we have $p_c = 1/2$.

Percolation Strength

Percolation strength of an infinite cluster is the probability of any arbitrary site to be the part of the infinite cluster. For the sake of calculation, for $p > p_c$ in the Bethe lattice, we introduce a new quantity Q as the probability that an arbitrary site is note connected to the infinite cluster through a fixed branch originating from this site. Restricting ourselves to the lattice with $z = 3$ and using basic probability theory, the strength

$$P(p) = p(1 - Q^3) \quad (4.54)$$

Here p is the probability that the site is occupied and $(1 - Q^3)$ is the probability that at least one branch is connected to infinity.

The probability that the two subbranches which start at the neighbor are not both leading infinity is Q^2 . The quantity pQ^2 is the probability that this neighbor is occupied but not connected to infinity by any of its two subbranches. This neighbor is empty with probability

$(1 - p)$, in which case even well connected subbranches do not help it. This gives us,

$$Q = (1 - p) + pQ^2 \quad (4.55)$$

This is the probability that this fixed branch does not lead to infinity, either because the connection is already broken at the first neighbor, or because later something is missing in the subbranch. So the solution of this quadratic equation is

$$Q = 1, \frac{1-p}{p} \quad (4.56)$$

For z neighbors, in general we have

$$Q = 1, 1 - \frac{2p(z-1) - 2}{p(z-1)(z-2)} \quad (4.57)$$

for $p < p_c$, there are no infinite clusters, fo with probability 1 there are no connection to infinity. Now we use Taylor expansion for $P(p)$ around $p = p_c = 1/2$

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p \left(1 - \left(\frac{1-p}{p}\right)^3\right) & \text{for } p \geq p_c \end{cases} \quad (4.58)$$

Let,

$$f(p) = \left(\frac{(1-p)}{p}\right)^3 \quad (4.59)$$

Then

$$\begin{aligned} f'(p) &= -3p^{-4}(1-p)^3 - 3p^{-3}(1-p)^2 \\ &= -\frac{3}{p} \left(\frac{(1-p)}{p}\right)^3 - \frac{3}{p} \left(\frac{(1-p)}{p}\right)^2 \end{aligned} \quad (4.60)$$

$$P(p) = P(p_c) + (p - p_c)P'(p_c) + \dots \quad (4.61)$$

$$= 0 + (p - p_c)(1 - f(p_c) - pf'(p_c)) + \dots \quad (4.62)$$

$$= 6(p - p_c) + \dots \quad (4.63)$$

$$(4.64)$$

Therefore we get

$$P(p) \propto (p - p_c) \text{ for } p \rightarrow p_c^+ \quad (4.65)$$

the critical exponent β is defined by

$$P(p) \propto (p - p_c)^\beta \quad (4.66)$$

Thus in Bethe lattice $\beta = 1$.

Mean Cluster Size

In case of Bethe lattice the mean cluster size is defined as the average number of sites to which the origin belongs. Let T be the mean cluster size for one branch, that is the average number of sites to which the origin is connected and which belongs to one branch. Again, subbranches have the same mean cluster T as the branch itself. If the neighbor is empty the cluster size for this branch is zero. If the neighbor is occupied, it contributes its own mass to the cluster which is unity and adds the mass T for each of its two subbranches. Thus,

$$T = (1 - p) \times 0 + p(1 + 2T) \quad (4.67)$$

Solving this we get

$$T = \frac{p}{1 - 2p} \quad (4.68)$$

for $p < p_c$.

The total cluster size is zero if the origin is empty and $(1 + 3T)$ if the origin is occupied.

Therefore the mean cluster size $S(p)$ is

$$S(p) = 1 + 3T \quad (4.69)$$

$$\begin{aligned} &= \frac{1+p}{1-2p} \\ &= \frac{1+p}{2(p_c - p)} \\ &= \frac{1+p}{2}(p_c - p)^{-1} \end{aligned} \quad (4.70)$$

Thus the critical exponent $\gamma = 1$ for Bethe lattice. This is the exact result for mean cluster size and we notice that it diverges for $p \rightarrow p_c$.

Correlation Function and Correlation Length

The radial correlation function $g(r)$ is the average number of occupied sites within the same cluster at a distance r from an arbitrary occupied site. The probability that a site at distance r from the origin is occupied and the sites in between are occupied too is equal to p^r . Now if we think about a shell of radius r then the number of all the sites enclosed by this shell is $z(z-1)^{r-1}$. Thus

$$g(r) = z(z-1)^{r-1} p^r \quad (4.71)$$

$$= \frac{z}{z-1} (p(z-1))^r \quad (4.72)$$

$$= \frac{z}{z-1} \exp [\log [p(z-1)]] \quad (4.73)$$

The value of percolation threshold for Bethe lattice can be found by analyzing the behaviour of the correlation function at large distances, i.e. at $r \rightarrow \infty$. For $p(z-1) < 1$, $g(r)$ decreases exponentially, on the other hand for $p(z-1) > 1$, the correlation function diverges which signifies the existence of an infinite cluster. Mathematical treatment yields the correlation

length from (4.34)

$$\begin{aligned}\xi &= \frac{-1}{\log[p(1-z)]} \\ &= \frac{-1}{\log(p/p_c)} \\ &= (p - p_c)^{-1}\end{aligned}\tag{4.74}$$

as p approaches p_c , that is $v = 1$.

Clearly the 1D lattice and Bethe lattice exhibits power law while we approach a critical value which suggests the same phenomena in other variants of such problems.

4.8 Algorithm

In the classical Hosen-Kopelman algorithm for percolation model [67], one first choose an occupation probability p and then generate a number r for each site of the lattice. The site is occupied if $r \leq p$ and remain empty if $r > p$. One therefore create an entire new state of a given lattice size for every different value of p . Note that the number of occupied sites n for a given p may vary in each realization. However, the expected or ensemble average over M experiments will give $n = pM$ in the limit $M \rightarrow \infty$. Thus the number of occupied bonds or sites is also a measure of p . Using this idea Ziff and Newman [98] proposed an algorithm which generate states for each value of n from zero up to some maximum value $n = L^2$ for site percolation on $L \times L$ square lattice for instance. In this way, one can save some effort by noticing the fact that a new state with $n + 1$ occupied sites or bonds can be created by adding one extra randomly chosen site or bond to the state containing n sites or bonds. The first step of their algorithm is to decide an order in which the bonds or sites are to be occupied. That is, every attempt to occupy a bond/site is successful.

4.8.1 Square Lattice

A square lattice is an ideal playground for percolation. A square lattice of linear size L has L^2 sites connected by $2L^2$ bonds with periodic boundary condition and by $2L(L - 1)$ bonds without periodic boundary condition. All sites are equally separated from each other at a

certain distance. And all sites have exactly four neighbor. Since with the periodic boundary condition the sites in the left edge are connected with the sites in the right edge and same rule for sites in the top and bottom edges. We always want our experimental result in the thermodynamic limit. This means that we want the results for a lattice where $L \rightarrow \infty$. In other words the sites are densely spaced. But that is practically impossible. The simple solution to this problem is to use number of large lengths, (say $L = \{L_1, L_2, \dots, L_n\}$, where n is a finite number and $L_1 < L_2 < \dots < L_n$), and extrapolate the results for infinite lattice. The visual structure of the square lattice is as follows (4.10a). This is an empty lattice structure. Filled circles are for occupied site and filled bonds are for occupied bonds (4.10).

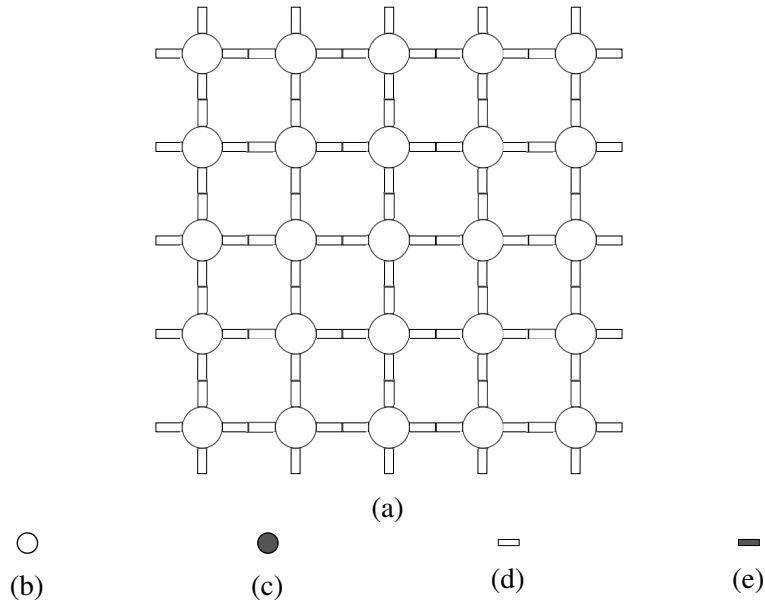


Fig. 4.10 (a) Square Lattice (empty skeleton) of length $L = 5$ where all sites and bonds are empty (b) Empty site (c) Occupied site (d) Empty bond (e) Occupied bond.

Percolation is known as site or bond type depending on whether we occupy sites or bonds respectively. Here we describe bond percolation process in detail and site percolation in brief.

4.8.2 Bond Percolation

One of the famous percolation type is random bond percolation on square lattice. Here we assume that all the labeled bonds are initially frozen. The rule is then to choose one frozen bond at each step randomly with uniform probability and occupy it. We continue

the process one by one till the occupation probability p , fraction of the total bonds being occupied, reaches to unity. At $p = 0$ each site is a cluster of its own size and as p is tuned towards increasing p then we observe clusters, a group of sites connected by occupied bonds, are continuously formed and grown on the average. In the process there comes a critical state when occupation of just one more bond results in the emergence of a cluster that spans across the entire system for the first time. This process of cluster growth is shown in figure (4.11). Notice that if occupying a bond can be of two kind. one is intercluster connection where two

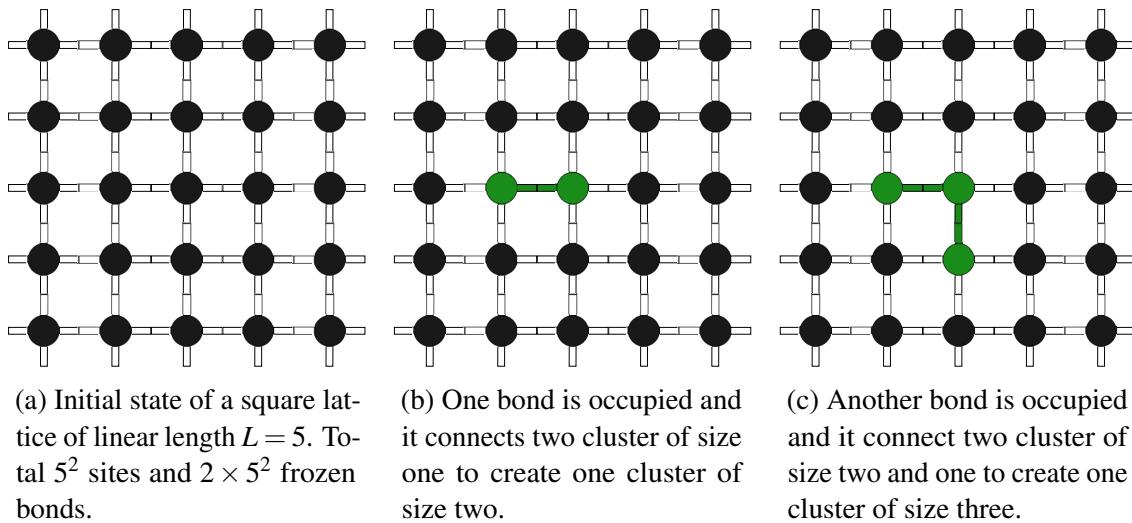


Fig. 4.11 Cluster growth in bond percolation in initial state.

distinct cluster is connected to form a larger cluster whose size is the sum of the connecting cluster. Another is the intracluster connection where two end of same cluster is connected but the cluster size remains invariant. Figure (4.12) demonstrate this process.

Using this process in mind we measure various quantity, for example Entropy, Spanning probability, Order Parameter etc., and the we use the scaling relation to obtain the exponents which is done in chapter (??) for site percolation.

4.8.3 Site Percolation

Here we discuss the traditional definition of site percolation and in section (5.1) we discuss what goes wrong if we use this definition and how we can resolve them in detail which is one of the purpose of this thesis.

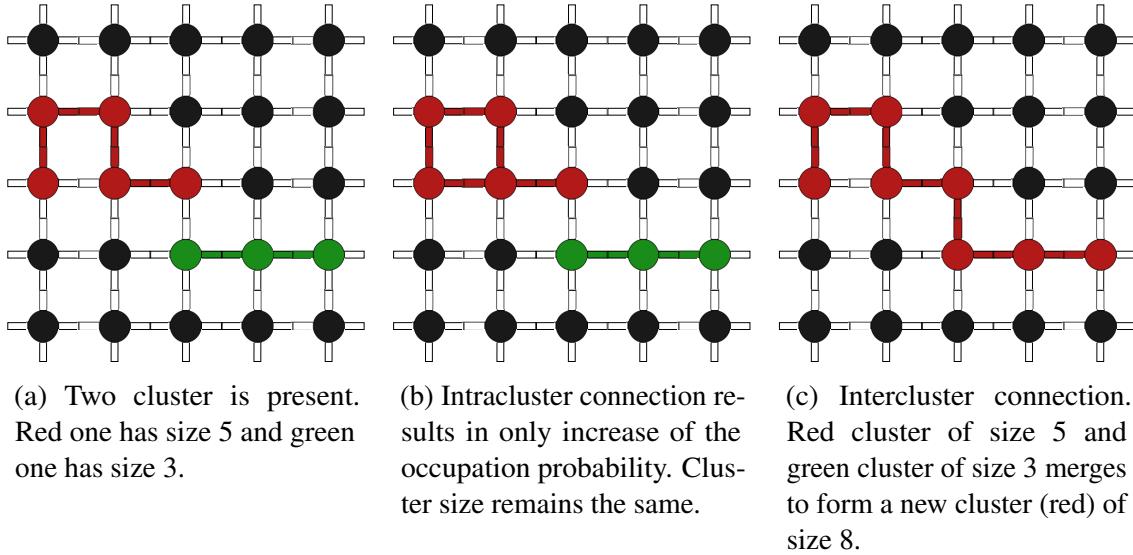


Fig. 4.12 Intercluster and intracluster connection.

Now in site percolation we take a square lattice of linear length L which have L^2 sites. We occupy each site with probability p and keep it empty with probability $(1 - p)$. Thus after we have visited all the sites in the lattice we get to measure any quantity of this system for probability p . Here we measure the cluster size by number of sites in the cluster as we do in bond percolation. In this way we get to measure a quantity for a fixed probability p in each realization which is the classical Hoshen-Koppelman (HK) algorithm [67].

Instead we use Newman-Ziff algorithm so that we can measure various observable quantities over the entire range of p in every realization instead of measuring them for a fixed probability p in each realization [98]. In NZ algorithm we pick a site at random with uniform probability and occupy it. Thus if we occupy n sites we get a system with occupation probability $p = n/N$ where $N = L^2$. This process is further discussed in the next section (4.8.4).

4.8.4 Newman-Ziff (NZ) algorithm

To study random percolation, we use Newman-Ziff (NZ) algorithm as it helps calculating various observable quantities over the entire range of p in every realization instead of measuring them for a fixed probability p in each realization [98]. On the other hand, in classical Hoshen-Koppelman (HK) we can only measure an observable quantity for a given p

in every realization and this is why NZ is more efficient than HK [67]. To illustrate the idea we consider the case of bond percolation first. According to the NZ algorithm, all the labelled bonds $i = 1, 2, 3, \dots, M$ are first randomized and then arranged in an order in which they will be occupied. Note that the number of bonds with periodic boundary condition is $M = 2L^2$. In this way we can create percolation states consisting of $n + 1$ occupied bonds simply by occupying one more bond to its immediate past state consisting of n occupied bonds. Initially, there are $N = L^2$ clusters of size one. Occupying the first bond means forming a cluster of size two (four). However, as we keep occupying thereafter, average or mean cluster size keep growing at the expense of decreasing cluster number. Interestingly, all the observables in percolation, this way or another, related to cluster size and hence proper definition of cluster is crucial. One of the advantages of the NZ algorithm is that we calculate an observable, say X_n , as a function of the number of occupied bonds (sites) n and use the resulting data in the convolution relation

$$X(p) = \sum_{n=1}^N p^n (1-p)^{N-n} X_n, \quad (4.75)$$

to obtain $X(p)$ for any value of p . The appropriate weight factor for each n at a given p is $\sum_{n=1}^N p^n (1-p)^{N-n}$ [98]. The convolution relation takes care of that weight factor and hence helps obtaining a smooth curve for $X(p)$.

The detail discussion of the use of convolution relation and how we can efficiently implement in a program is discussed in Appendix (B).

4.9 Application

Ever since the percolation phenomena was discovered it has been extensively used in wide range of science. Some of it is discussed here. Though limited, this discussion gives us the significance of percolation and enables us to appreciate it.

4.9.1 Epidemiology

Many diseases spread through human populations via close physical interactions. The interpersonal contact patterns that underlie disease transmission can naturally be thought to form a network, where links join individuals who interact with each other. During an outbreak,

disease then spreads along these links. All epidemiological models make assumptions about the underlying network of interactions, often without explicitly stating them.

Percolation has long been an important tool in infectious disease epidemiology [15]. L Meyers gave a wonderful insight of contact network epidemiology, a more powerful approach that applies bond percolation on random graphs to model the spread of infectious disease through heterogeneous populations [91].

Before that in 2000, Moore et al. studied some simple models of disease transmission on small-world networks [93]. They showed that the resulting models display epidemic behavior when the infection or transmission probability rises above the threshold for site or bond percolation on the network, and they gave exact solutions for the position of this threshold in a variety of cases.

Alessandro Vespignani and his team studied wifi networks and malware epidemiology. They developed an epidemiological model that takes into consideration prevalent security flaws on these routers. They simulated spread of such a contagion on real-world data for georeferenced wireless routers [69].

Sander et al. considered a spatial model related to bond percolation for the spread of a disease that includes variation in the susceptibility to infection. They worked on a lattice with random bond strengths and showed that with strong heterogeneity, i.e. a wide range of variation of susceptibility, patchiness in the spread of the epidemic is very likely, and the criterion for epidemic outbreak depends strongly on the heterogeneity. Their results were qualitatively different from those of standard models in epidemiology, but correspond to real effects [114].

After the birth of scale free network the study of epidemics has become even more popular among statistical physicists.

4.9.2 Neural Network and Cognitive Psychology

Percolation is used to understand the way activation and diffusion of neural activity occur within neural networks [57]. Iian Breskin's team in 2006 studied living neural networks by measuring the neurons' response to a global electrical stimulation. They showed through analysis that neural connectivity is lowered by reducing the synaptic strength, chemically blocking neurotransmitter receptors. They used a graph-theoretic approach to show that

the connectivity undergoes a percolation transition. This occurs as the giant component disintegrates, characterized by a power law with an exponent $\beta \simeq 0.65$ [26].

It is easiest to understand percolation theory by explaining its use in epidemiology [93]. Individuals that are infected with a disease can spread it knowingly or unknowingly via social or physical interaction. It's easy to say that the more social a person is the more it is likely that he will spread more disease than the unsocial one. Therefore some factors, e.g., occupation, size of social circle etc, influence the rate of infection.

Now, if one were to think of neurons as the individuals and synaptic connections as the social bonds between people, then one can determine how easily messages between neurons will spread [57] When a neuron fires, the message is transmitted along all synaptic connections to other neurons until it can no longer continue.

Synaptic connections are considered either open or closed (like a social or unsocial person) and messages will flow along any and all open connections until they can go no further. Just like occupation and sociability play a key role in the spread of disease, so does the number of neurons, synaptic plasticity [71] and long-term potentiation when talking about neural percolation. Percolating clusters are a single large group of neurons that are all connected by open bonds and take up the majority of the network. Any signals that originate at any point within the percolating cluster will have a great impact and diffusion across the network than signals that original outside of the cluster. This is much like how a teacher is more likely to spread an infection to a whole community through contact with the students and subsequently with the families than an isolated businessman that works from home.

4.9.3 Ferromagnetism

One of the most studied phase transition phenomena of physics is that para-magnetic to ferromagnetic transition. The magnetic spins of a magnetic material, e.g., nickel, interact with each other: the energy is lower if the two spins on adjacent nickel atoms are parallel than if they are anti-parallel. This lower energy tends to cause the spins to be parallel and below a temperature called the Curie temperature, T_c , most of the spins in the nickel are parallel, their magnetic moments then add up constructively and the piece of nickel has

a net magnetic moment: it is a ferromagnetic. Above the Curie temperature on average half the spins point in one direction and the other half in the opposite direction. Then their magnetic moments cancels out, and the nickel has no net magnetic moment. It is then a para-magnet. Thus at T_c the nickel goes from having no magnetic moment to having a magnetic moment. This is a sudden qualitative change and when this happens we say that a phase transition has occurred. Here the phase transition occurs when the magnetic moment goes from zero to non-zero. It is from the para-magnetic phase to the ferromagnetic phase. So, this critical value T_c of the temperature marking the borderline between the existence and non-existence of so called spontaneous magnetization. A standard mathematical model for this phenomenon is the Ising model [35]. It turns out that there are two parameters which specify the conditional probabilities: the 'external magnetic field' h , and the strength J of interaction between neighbors. If $J = 0$, the states of different vertices are independent, and the process is equivalent to site percolation [39]. The relationship between the Ising model and bond percolation is rather strong. It turns out that they are linked via a type of 'generalized percolation' called the other considerations [38, 118]. Studing the random-cluster model, one can obtain conclusions valid simultaneously for percolation and the Ising model. This discovery was made in 1970 by Fortuin and Kastelyn [56, 54, 55], and it has greatly influenced part of the current view of disordered physical systems

4.9.4 Cosmology

We know mass distribution and motions of the components of a galaxy are determined by gravity, it has not been clear what is responsible for the striking morphology of a spiral galaxy such as shown in the figure. The spiral arms extend over 16,000 parsecs (1 parsecs equals 3.26 light-years), and the traditional view is that it is necessary to have a long-range interaction like gravity, which interacts with object that have mass, to create such long-range order. However, in condensed matter physics it is well known that long-range order can be induced by a short-range interaction, and this is a characteristic feature of a continuous phase transition [48].

The structural features of spiral galaxies arises from a percolation phase transition that underlies the phenomenon of propagating star formation. According to this view, the



Fig. 4.13 NGC 4414, a typical spiral galaxy in the constellation Coma Berenices, is about 55,000 light-years in diameter and approximately 60 million light-years away from Earth.

appearance of spiral arms is a consequence of the differential rotation of the galaxy and the characteristic divergence of correlation lengths for continuous phase transitions.

Other structural properties of spiral galaxies, such as the distribution of the gaseous components and the luminosity, arise directly from a feedback mechanism that pins the star formation rate close to the critical point of the phase transition. At least for some galaxies, morphological and other features are already fixed by general properties of phase transitions, irrespective of detailed dynamic or other considerations [118, 38].

4.9.5 Others

Percolation model has also been applied to a wide variety of natural and social phenomena such as the spread of disease in a population [95], flow of fluid through porous media [41], conductor-insulator composite materials [90], resilience of systems [11, 103], dilute magnets [18], the formation of public opinion [129, 122, 94] and spread of biological and computer viruses leading to epidemic [96, 93]

Chapter 5

Ballistic Deposition With Redefinition of Site Percolation

Here we first revisit random site and bond percolation in square lattice focusing primarily on entropy which quantifies the degree of disorder and order parameter that measures the extent of order. Note that being two opposite quantities they can neither be minimum nor be maximum at the same time which is perfectly consistent with bond percolation. However, the same is not true for traditional site percolation as we find that entropy and order parameter are both zero at occupation probability $p = 0$ and the way entropy behaves it violates the second law of thermodynamics. To overcome this we redefine the site percolation where we occupy sites to connect bonds and we measure cluster size by the number of bonds connected by occupied sites. This resolves the problem without affecting any of the existing known results whatsoever.

Then we investigate percolation by random sequential ballistic deposition (RSBD) on a square lattice with interaction range upto second nearest neighbors. The critical points p_c and all the necessary critical exponents $\alpha, \beta, \gamma, \nu$ etc. are obtained numerically for each range of interactions. Like in its thermal counterpart, we find that the critical exponents of RSBD depend on the range of interactions and for a given range of interaction they obey the Rushbrooke inequality. Besides, we obtain the fractal dimension d_f that characterizes the spanning cluster at p_c (4.6.7). Our results suggest that the RSBD for each range of interaction

belong to a new universality class which is in sharp contrast to earlier results of the only work that exist on RSBD.

5.1 Redefinition of Site Percolation

we first define the percolation process and to do it we first need to choose a skeleton. It can either be an abstract graph which is now better known as network or be a spatially embedded lattice which are consist of nodes or site and links or bonds. A square lattice of linear size L has L^2 sites connected by $2L^2$ bonds with periodic boundary condition and by $2L(L - 1)$ bonds without periodic boundary condition. Percolation is known as site or bond type depending on whether we occupy sites or bonds respectively. In section (4.8.2) we have described the bond percolation and we have seen that we occupy bond to connect clusters of different sizes.

Interestingly, we find that the way the relative size of the spanning cluster $P = s_{\text{span}}/N$ varies with p such that $P = 0$ for $p \geq p_c$ and $P \sim (p - p_c)^\beta$. This is reminiscent of the order parameter of continuous phase transition and hence P is regarded as the order parameter for percolation [123, 19]. This is one of the reasons why scientists in general and physicists in particular find percolation theory so attractive.

We still have many unresolved issues in percolation. For instance, we know that the order parameter measures the extent of order but we do not yet know what order really is in percolation. Note that $P = 0$ in the entire disordered phase at least in the thermodynamic limit. We therefore need another quantity that can quantify the degree of disorder in the disordered phase. The obvious choice is entropy without which any model for phase transition is incomplete since, like order parameter, it is also used to define the order of transition. In the case of first order transition, entropy is discontinuous at the critical point and the corresponding gap is proportional to the latent heat. Despite being such an important quantity, its definition remained elusive in percolation until our recent work in 2017 [65, 110]. Note that both entropy and the order parameter cannot be minimally low or maximally high at the same time since no system can be in the ordered and disordered at the same time. Thus, they form such a pair that when one is minimally low the other has to be maximally high and vice versa. Moreover, the two quantities together characterize whether the transition

is accompanied by symmetry breaking or not. Recall that in the continuous thermal phase transition, such as paramagnetic to ferromagnetic transition, the order parameter is maximum, $m \rightarrow 1$ as temperature $T \rightarrow 0$, where entropy is minimum there. On the other hand, the order parameter is zero or minimum where the entropy is maximally high. Meanwhile at and near the critical point both the quantities undergo an abrupt change. It implies that the paramagnetic to ferromagnetic transition is an order-disorder transition which also means that the transition is accompanied by symmetry breaking.

5.1.1 Definition of Entropy and Order Parameter

The two most important quantities of interests in the theory of phase transition and critical phenomena are the entropy H and the order parameter P since they are the ones which define the nature of transition. In the first order or discontinuous phase transition, entropy must suffer a jump or discontinuity at the critical point which is why first order transition requires latent heat. Similarly, the order parameter too must suffer a jump or discontinuity at the critical point and that is the why new and old phase can coexist at the same time in the first order transition. Besides, they are also used as a litmus test to check whether the transition is accompanied by symmetry breaking or not. In the case of symmetry breaking, the system undergoes a transition from the disordered state, which is characterized by maximally high entropy, to the ordered state, which is characterized by maximally high order parameter. Such transition happens with an abrupt or sudden change in P and H but without gap or discontinuity at p_c . Percolation being a probabilistic model for phase transition, there is absolutely no room for considering thermal entropy. To this end, the best candidate is definitely the Shannon entropy

$$H(t) = -K \sum_i^m \mu_i \log \mu_i, \quad (5.1)$$

where we choose $K = 1$ since it merely amounts to a choice of a unit of measure of entropy [121].

On the other hand, the strength $P(p, L)$ of the spanning cluster for system size L is defined as

$$P = \frac{\text{Number of bonds in the spanning cluster}}{\text{Total number of bonds} = 2L^2}. \quad (5.2)$$

Essentially, it describes the probability that a site picked at random belongs to the spanning cluster at occupation probability p for system size L . It has been found that in the limit $L \rightarrow \infty$ the probability $P(p, L) = 0$ for $p \leq p_c$ and it reaches to its maximum value $P(p, L) = 1$ following power-law $P \sim (p - p_c)^\beta$ near but above p_c . This is reminiscent of the order parameter in the continuous thermal phase transition like magnetization during the ferromagnetic transition. However, for finite system size $P(p, L)$ may have non-zero value at $p < p_c$. However, as we increase the size L of the system it always shows a clear sign of becoming zero. There exists yet another definition where we can use the size of the largest cluster instead of the spanning cluster. Note that both the definitions behave in the same fashion and have all the properties of the order parameter. That is, in the limit $L \rightarrow \infty$, $P = 0$ for $p \leq p_c$ and it rises from $P = 0$ at p_c to $P = 1$ continuously and monotonically like $P \sim (p - p_c)^\beta$. Such behavior is reminiscent of order parameter like magnetization m in the ferromagnetic transition and hence P is regarded as the order parameter in percolation theory.

5.1.2 Problem for entropy with traditional site percolation

We first measure entropy for random bond percolation where initially every site is a cluster of its own size. As we keep occupying or reactivating frozen bonds, clusters are continuously formed and their sizes on average are grown. Consider that at an arbitrary step of the process there are m distinct, disjoint, and indivisible labelled clusters $i = 1, 2, \dots, m$ whose sizes are s_1, s_2, \dots, s_m respectively. We can therefore define $\mu_i = s_i / \sum_i s_i$ as the corresponding cluster picking probability (CPP), that a site picked at random belongs to the cluster i , which is naturally normalized $\sum_j s_j = N$ [65, 64]. Thus, at $p = 0$ we have $\mu_i = 1/N$ for all the sites $i = 1, 2, \dots, N = L^2$ which is exactly like the state of the isolated ideal gas where all the allowed microstates are equally likely. It is thus expected that entropy is maximum $H = \log N$ at $p = 0$ revealing that we are in a state of maximum uncertainty just like the state of the isolated ideal gas. On the other hand, as we go to the other extreme at $p = 1$ we find that all the sites belong to one cluster that makes $\mu_1 = 1$. It implies that entropy is zero at $p = 1$ and hence we are in a state of zero uncertainty just like the perfectly ordered crystal structure. In order to see how entropy interpolates between $p = 0$ and $p = 1$, we use CPP in Eq. (5.1) and the resulting entropy is shown in Fig. (5.1a) as a function of p for different system size.

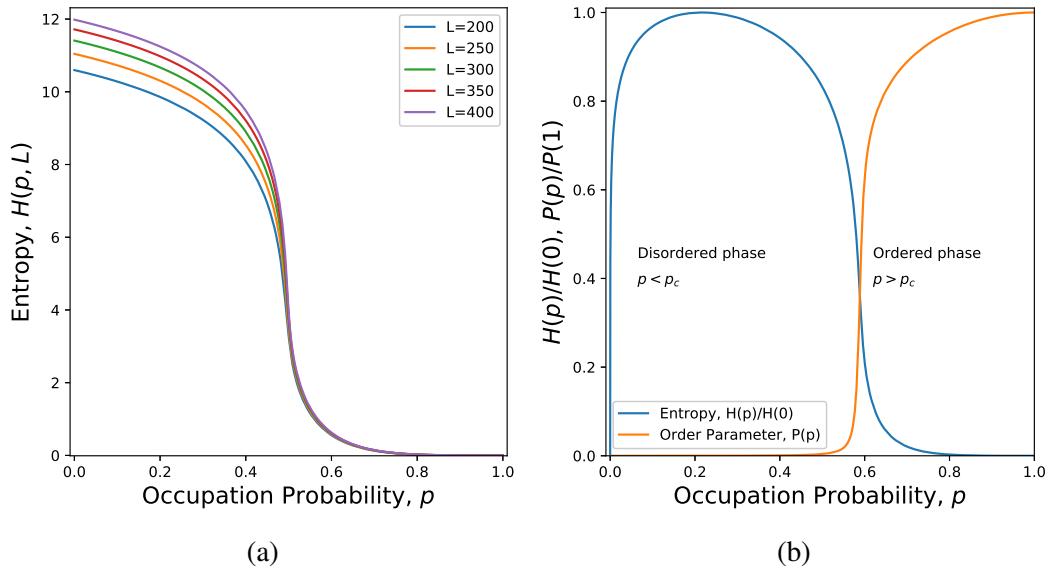


Fig. 5.1 (a) Entropy H versus t for bond percolation. (b) Entropy (blue) and order parameter (orange) for traditional site percolation. we plot entropy $H(p)/H(0)$ and order parameter $P(p)/P(1)$ in the same graph to see the contrast.

To see how entropy for random site percolation differs from that of the bond type we now measure entropy for traditional definition of site percolation. In this case, it is assumed that initially all the sites are frozen or empty. The process starts with occupation of sites one by one at random and measure the cluster size exactly like in the bond percolation. It means initially CPP does not exist and after the occupation of the first site $\mu = 1$ and hence entropy $H = 0$ at $p = 1/N$ which is essentially zero in the limit $N \rightarrow \infty$. As we further occupy sites, we observe a sharp rise in the entropy to its maximum value, see Fig. (5.1b), which happens near $p = 0.2$. Thereafter it decreases with p qualitatively in the same way as in the case of random bond type percolation. To see the contrast we also show the order parameter also in Fig. (5.1b). This figure suggest that at $p \sim 0$ entropy and order parameter both are zero which cannot be true. Besides, entropy of site percolation violates the second law of thermodynamics as it states that entropy of isolated system cannot first increase and then decrease again. It thus warrants redefinition of site percolation.

5.1.3 Site percolation re-defined

The question is: How can we resolve the problem with the definition of traditional site percolation? We can get the definition of site percolation from the definition of bond percolation simply by replacing bonds with site and vice versa. That is, we assume that initially isolated bonds are already there in the system which are shown in Fig. (5.2) by the thick black lines and sites are empty (white circles). We then keep picking one site at each step with uniform probability and occupy it to connect four bonds around it.

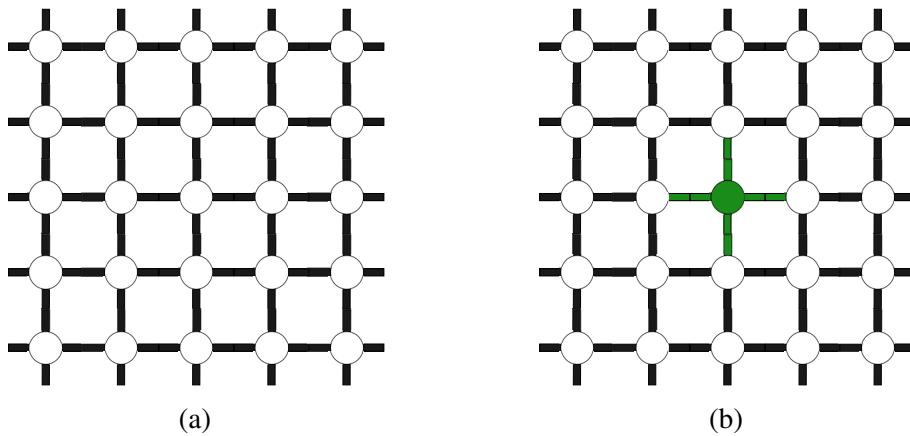


Fig. 5.2 (a) Illustration of redefined site percolation on square lattice. We assume that process starts with isolated bonds (thick black lines) but sites are empty (white circles). (b) Occupying one site connects four bonds hence it forms a cluster of size four.

We measure cluster size by the number of bonds that it contains and occupation probability as the fraction of the sites being occupied. For instance, the cluster of size four is shown in Fig. (5.2b) by green color. Using this renewed definition, we again measure entropy and find entropy is just like its bond counterpart. That is, entropy is maximum at $p = 0$ and as p approaches p_c it drops sharply. It then again decreases slowly to zero as p reaches its maximum value $p = 1$ which is shown in Fig. (5.3a). We clearly see that its qualitative behaviour is exactly the same as Fig. (5.1a) for the bond percolation and hence the problem of absurdity, that entropy and order parameter both equal to zero at $p = 0$, and the violation of the second law of thermodynamics are resolved.

Perhaps plots of entropy and order parameter in the same graph can help us appreciate their opposing nature better than they are shown separately. Note that the numerical value of the maximum entropy, which is equal to $\log(N)$, is much higher than the maximum value of

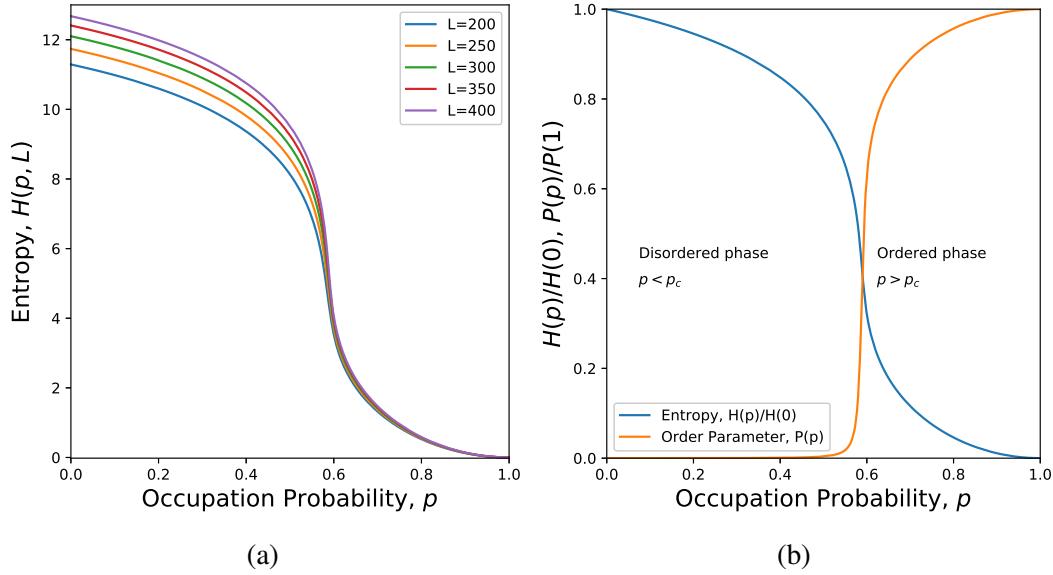


Fig. 5.3 For redefined site percolation we plot (a) Entropy. (b) Entropy $H(t)/H(0)$ and order parameter $P(t)/P(1)$ in the same graph to see the contrast. It can be easily seen that $P = 0$ where entropy is maximally high and order parameter is maximally high where entropy is minimally low which is reminiscent of order-disorder transition in the ferromagnetic transition.

P which is equal to one. We, therefore, measure relative entropy $H(p)/H(0)$ and relative order parameter $P(p)/P(1)$ in an attempt to re-scale their values so that in either cases their respective maximum values become unity. The plots of re-scaled entropy and order parameter are shown in Fig. (5.3b) which clearly shows that H is maximally high where $P = 0$ and the order parameter is maximally high where H is minimally low. Besides, they both undergo a sharp change in the vicinity of the critical point p_c and consistent with the second law of thermodynamics. This is exactly what is expected as order parameter measures the extent of order and entropy quantifies the degree of disorder. It means that percolation transition is accompanied by symmetry breaking just like paramagnetic to ferromagnetic transition. In other words it is an order-disorder transition since in one phase $P = 0$ and H is maximally high revealing it corresponds to disordered phase and in the other phase P is maximally height but H is minimally low revealing it is the ordered phase.

5.1.4 Is site-bond universality still valid?

We now check if the re-defined site percolation still gives the same critical point $p_c = 0.5927$ and the same the critical exponent ν of the equivalent counterpart of the coorelation length or not. The best quantity for finding the critical point p_c and critical exponent ν is the spanning probability $W(p)$. It describes the likelihood of finding a cluster that spans across the entire system either horizontally or vertically at a given occupation probability p . In Fig. (5.4a) we show $W(p)$ as a function of suitable class of width Δp which is essentially the plot os $W(p)$ as a function of p for different system sizes L . One of the significant features of such plots is that they all meet at one particular value regardless of the value of L . It is actually the critical point $p_c = 0.5927$ which is exactly the same known value as for the traditional definition of site percolation.

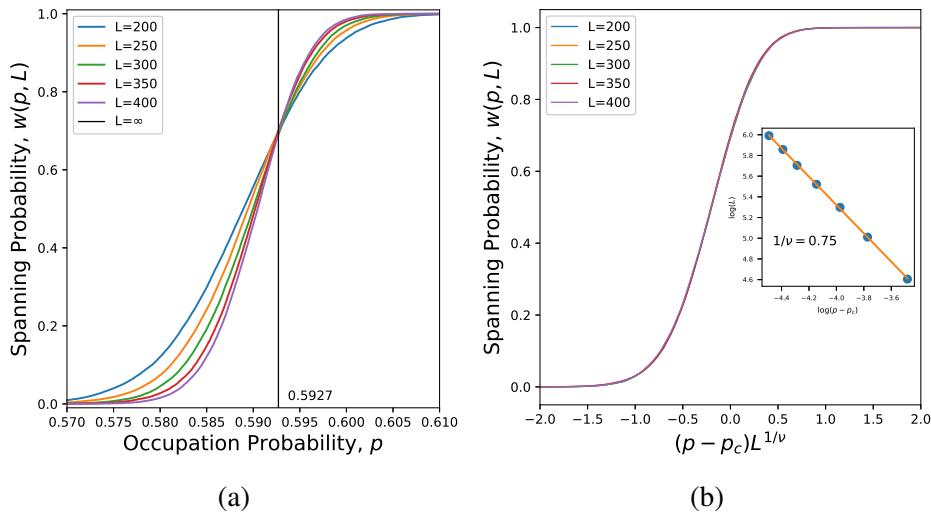


Fig. 5.4 (a) Spanning probability $W(p, L)$ vs p for different lattice sizes using new definition of site percolation. In (b) we plot dimensionless quantities W vs $(p - p_c)L^{1/\nu}$ using known value of $\nu = 4/3$ and find excellent data-collapse which is a proof that bond-site still belong to the same universality class.

Thus, the value of p_c does not depend on whether we measure the cluster size in terms of the number of sites or the number of bond it contains. Note that finding the p_c value for different skeletons is one of the central problems in percolation theory [136, 137]. To check whether the ν value is still the same we use its standard known value $\nu = 4/3$ [135]. We then plot of $W(p)$ vs $(p_c - p)L^{1/\nu}$ and find that all the distinct curves of Fig. (5.4a) collapse

into a universal scaling curve as shown in Fig. (5.4b) for $v = 4/3$. This is a clear testament that the critical point v is also the same as that of the traditional site percolation.

Next we attempt to find the critical exponent β of the order parameter P using the new definition of site percolation. First we plot order parameter $P(p)$ in Fig. (5.5a) as a function of p for different lattice size L . We now use the standard known values for $v = 4/3$ and $\beta/v = 0.104$ and plot $P(p,L)L^{\beta/v}$ versus $(p - p_c)L^{1/v}$ in Fig. (5.5b). We get an excellent data collapse revealing that the new definition of site percolation reproduces the known value of $\beta = 0.1388$ in $2d$ random percolation. It confirms that the site-bond universality is not affected by the new definition. Recently, we have also studied random percolation on scale-free lattice and found that $\beta = 0.222$ [64]. This is the only exception that, despite the dimension of the embedding space of the scale-free weighted planar stochastic lattice is two, yet it belongs to different universality class.

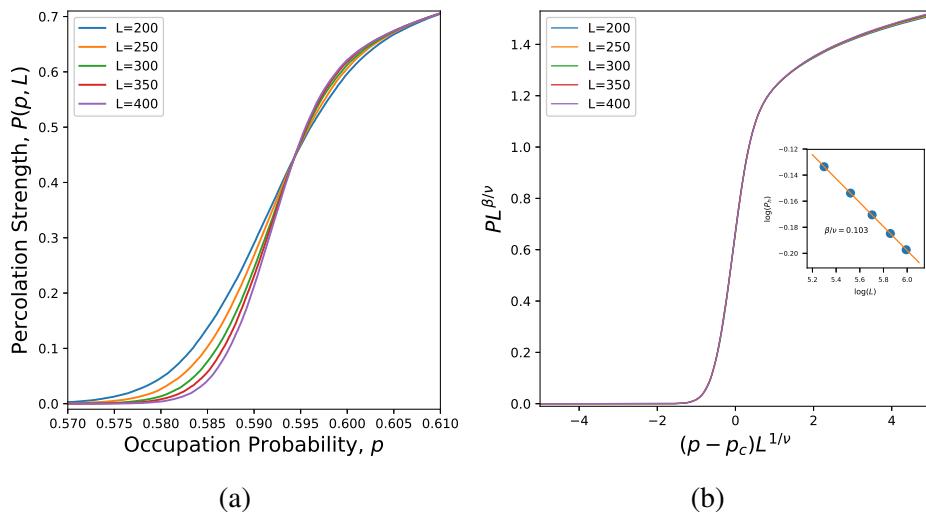


Fig. 5.5 (a) Order parameter $P(p,L)$ vs p for re-defined site percolation in the square lattice. (b) We plot $P(p,L)L^{\beta/v}$ versus $(p - p_c)L^{1/v}$ using know value of $v = 4/3$ and $\beta = 5/36$. An excellent data collapse proves that our way defining site percolation can still reproduce the same critical exponents.

Knowing the entropy pave the way of obtaining the specific heat since we know that it is proportional to the first derivative of entropy i.e. $C = TdS/dT$ where S is the thermal entropy. If we now know the exact equivalent counterpart of temperature then we can immediately obtain the specific heat for percolation. In our recent work we argued that $1 - p$ is the

equivalent counterpart of temperature and hence the specific heat for percolation is

$$C(p) = (1-p) \frac{dH}{d(1-p)}. \quad (5.3)$$

The plots of $C(p)$ as a function of p for different system size L is shown in Fig. (5.6a). We already know the value of $\alpha = 0.906$ from our recent work on bond percolation in the square lattice [65]. Using the the same values for α and v we plot $CL^{-\alpha/v}$ vs $(p - p_c)L^{1/v}$ in Fig. (5.6b) and find an excellent data collapse. It confirms that $\alpha = 0.906$ is indeed the same for both bond and redefined site percolation.

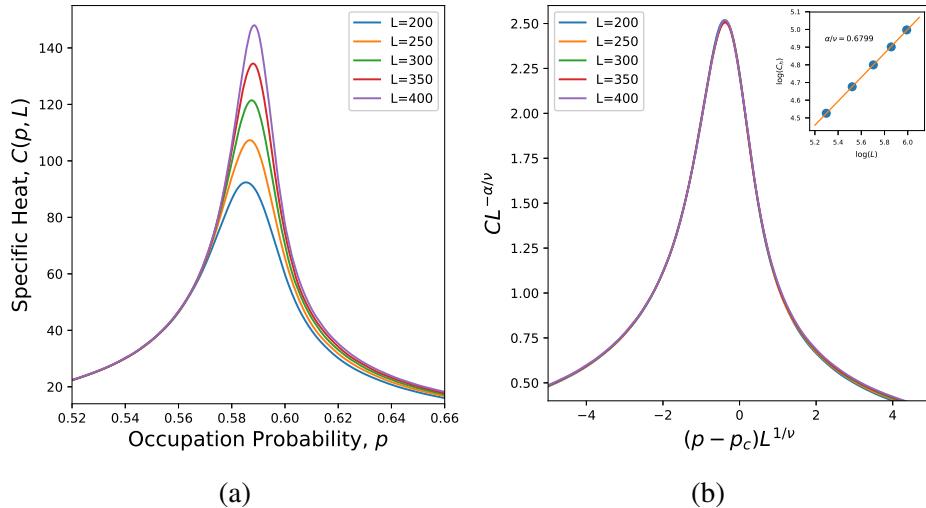


Fig. 5.6 Specific heat $C(p,L)$ vs p in square lattice for re-defined site percolation. In (b) we plot dimensionless quantities $CL^{-\alpha/v}$ vs $(p - p_c)L^{1/v}$ and we find an excellent data-collapse.

In percolation, yet another quantity of interest is the susceptibility. Traditionally, mean cluster size has been regarded as the equivalent counterpart of susceptibility. Sometimes variance of the order parameter $\sqrt{\langle P^2 \rangle - \langle P \rangle^2}$ too is regarded as susceptibility. Neither of the two actually gives respectable value for γ to obey the Rusbrooke inequality. Recently, we proposed susceptibility $\chi(p,L)$ for percolation as the ratio of the change in the order parameter ΔP and the magnitude of the time interval Δt during which the change ΔP occurs. Essentially it becomes the derivative of the order parameter P since $\Delta p \rightarrow 0$ in the limit $N \rightarrow \infty$ as $\Delta p = \frac{1}{2L^2}$. The idea of jump has been studied first by Manna in the context of explosive percolation [89]. The resulting susceptibility is shown in Fig. (5.7) as a function of p . We already know that $\gamma/v = 0.6407$ for bond percolation in the square lattice. Using the

same value for redefined site percolation in the plot of $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ we find that all the distinct curves in Fig. (5.7a) collapse superbly to give Fig. (5.7b). It implies once again that bond and redefined site percolation share the same γ value.

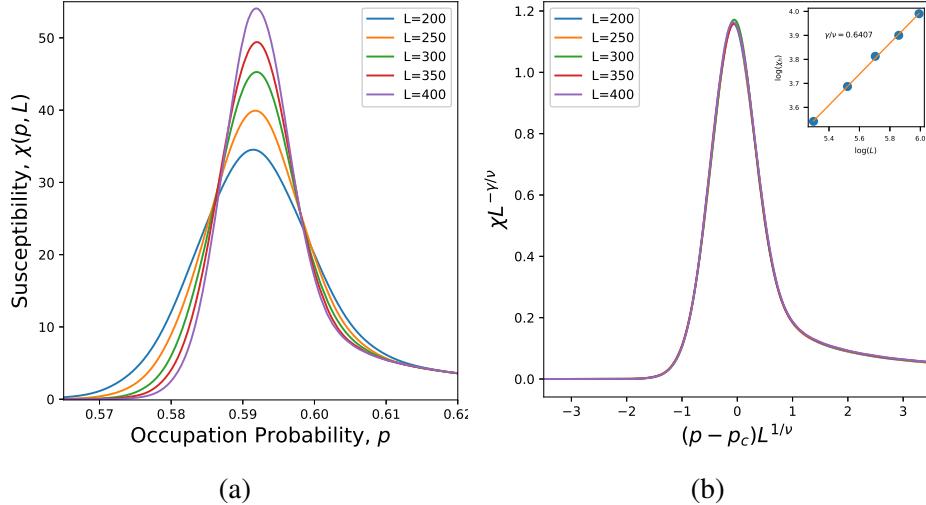


Fig. 5.7 (a) Plots of susceptibility $\chi(p)$ for redefined site percolation as a function of p in square lattice of different sizes. In (b) we plot dimensionless quantities $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ and we find an excellent data-collapse with $\gamma = 0.853$ which is the same as for bond type.

5.1.5 Fractal Dimension

At critical point the square lattice shows the property of a fractal [49] (4.6.7). We use the relation

$$S \sim L^{d_f} \quad (5.4)$$

taking log we get

$$\log(S) = d_f \log(L) \quad (5.5)$$

<<< HEAD Here S is the average size of the spanning cluster at critical point. Using this we get the figure (5.8). And we obtain fractal dimension d_f for L_0 which is listed in (6.3).
===== Here S is the average size of the spanning cluster at critical point. Using this we get the figure (??). And we obtain fractal dimension d_f for L_0 which is listed in (??). >>>
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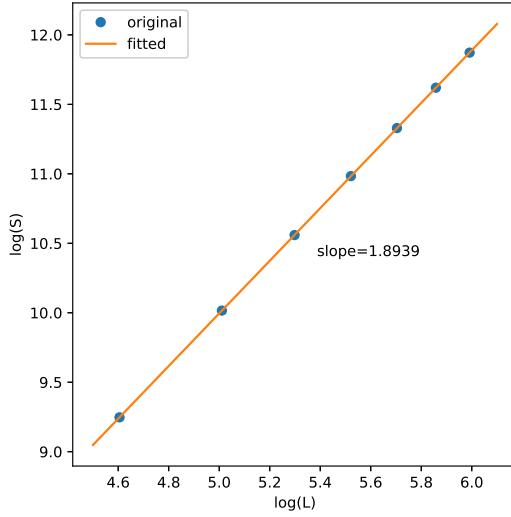


Fig. 5.8 We plot $\log(S)$ vs $\log(L)$ where S is the size of the spanning cluster and L is the length of the lattice. We obtain the slope 1.8939 which is the fractal dimensions of the system at p_c .

Fractal dimension gives us the information about the size of the spanning(wrapping) cluster. If the lattice size is known we can estimate the average size of the spanning cluster using d_f and (5.4).

5.2 Random Sequential Ballistic Deposition

Random sequential adsorption (RSA) refers to a process where particles are randomly introduced in a system, and if they do not overlap any previously adsorbed particle, they adsorb and remain fixed for the rest of the process. In RSA process we take a surface (say a lattice) and deposit particle (like hard sphere) there sequentially. Each particle cover a certain area and another particle cannot be in that area. Now if a particle is tried to be deposited in the occupied area it is simply rejected [4, 130]. In the ballistic deposition process, as in RSA, disks fall on a line with a uniform random distribution. However, unlike the RSA process, a disk landing on top of an adsorbed disk will not be immediately rejected [126].

Imagine a spherical shaped object, say marble, is thrown on top of a 2D square lattice structure. First possible scenario is that the marble will be deposited in the first encountered site in the lattice which is shown in figure (??). Now if the first encountered site is not empty, the possible scenario is that the marble will go in any of the four direction, $+x$, $-x$, $+y$

or $-y$, assuming no other direction in between is allowed in the lattice (??). Now if the first neighbor is not empty then the marble will continue to go on in the previously selected direction and choose the next neighbor. This is another topic of this thesis. Others have done some work in this topic [34, 126, 74, 128]. And we have found that for a different range of interaction model they all belong to different universality classes.

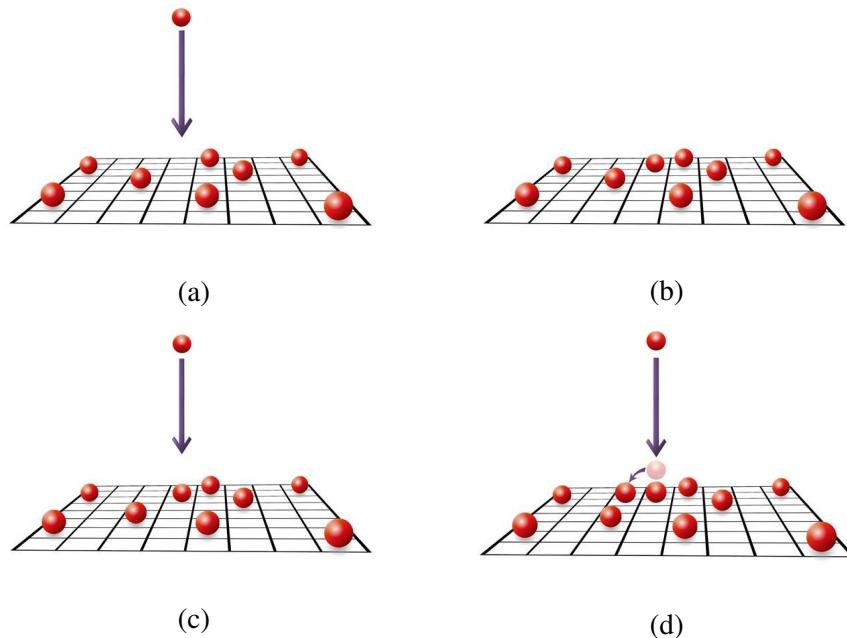


Fig. 5.9 (a)-(b) A schematic diagram to show if a particle fall on a randomly chosen empty site then it is straightaway absorbed there. (c)-(d) If the randomly chosen site is already adsorbed then the trial particle roll over it in one of the four direction at random. If it then find an empty site it is occupied else the attempt is rejected for L_1 . In the case of L_2 it goes one site further along the same line and then it is occupied if it finds an empty site else the trial attempt is permanently rejected.

In our experiment, we occupy a randomly chosen site if it is empty else we select one of its four neighbor to occupy if it is empty else select next neighbor in that direction and occupy that site if it is empty else ignore current iteration and choose another site randomly. This process is repeated until there is no empty site in the lattice. We call this process the ballistic deposition on the square lattice. We introduce 1st and 2nd nearest neighbor interaction in this way.

Random percolation (RP) model can also be seen as a random sequential adsorption (RSA) [74] process of particles on a given substrate to form monolayers of clusters of

complex shape and structures. In RSA, a site is first picked at random and it is occupied if it is empty and the trial attempt is rejected if it is already occupied. We shall first show that this process too reproduce all the existing results of the CRP including the p_c value. We can modify the rejection criterion. First, we assume that the adsorbing particles are hard sphere and impenetrable. Then we assume that if a particle fall onto an already adsorbed particle it is not straightaway rejected. Instead, it is allowed to roll down over the already deposited particle to one of its nearest neighbours at random following the steepest descent path. The particle is then adsorbed permanently if the nearest neighbour is empty else the trial attempt is rejected. This is known as the ballistic deposition (BD) [34, 126, 74, 128] model for L_1 . We also consider the case that if the nearest neighbour is occupied then the incoming particle attempt to push the neighbour to its next neighbour site along the same line to make room for itself. However, the trial attempt of pushing the neighbour is successful if the next neibouring site along the same line is empty else the trial attempt is discarded. We regard it as BD model for L_2 while the classical percolation correspond to BD model with L_0 . Our primary goal is to prove that the critical exponents of percolation changes as changes as we increase the range of interaction like we find in its thermal counterpart. We numerically find the various necessary critical exponents and find that BD for each different range of interaction belong to different universality class and each universality class obeys the Rusbrooke inequality.

Percolation is all about configuration of clusters of deposited particles and the investigation of the emergence of a large-scale connected path created by clusters formed by contiguous deposited particles. We use extensive Monte Carlo simulation on a square lattice with the usual periodic boundary condition to study site percolation according to RSBD rule.

The algorithm of the percolation by RSBD can be described as follows. We first label all the sites row by row from left to right starting from the top left corner. That is, we first label the first row from left to right as $i = 1, 2, \dots, L$, the second row again from left to right as $i = L + 1, L + 2, \dots, 2L$ and we continue this till we reach the bottom row which we label as $i = (L - 1)L + 1, \dots, L^2$. Then at each step we pick a discrete random number R from $1, 2, \dots, L^2 - 1, L^2$ using uniform random number generator and check if the site it represents is already occupied or not. If it is empty we occupy it straightaway and move on to the next

step. Else we pick one of its neighbours at random. The second attempt in the same step, that mimic the roll over mechanism, is successful if the neighbour it picks is empty and if not the trial attempt to deposit is rejected permanently and we move on to the next step anyway. This process is repeated over and over again till we want it to stop. We call it RSBD of degree one. We also consider the case of RSBS of degree two where the trial attempt is made to occupy the second nearest neighbour too. In this case if the incoming particle that fall onto an already occupied site and find its neighbour is occupied too but the next nearest neighbour site is empty then the neighbour move to the empty site to make space for the incoming particle to be deposited there.

In the following sections we study the threshold for L_1 and L_2 . Then we find out the critical exponents $\alpha, \beta, \gamma, \nu$ for L_1 and L_2 . We find that they all satisfy the Rushbrooke inequality which is listed in section (6). Then we find the fractal dimension of the system at threshold.

5.2.1 Critical occupation probability, p_c

When we occupy sites of the square lattice, initially, there are only clusters of size 1. As we keep occupying different size of clusters starts to appear. At a certain point a special cluster appears which spans the entire lattice. We call this cluster the *Spanning Cluster*. It should be noted that the spanning cluster is a special property of the lattice and the appearance of the spanning cluster is considered the phase transition. At the point where the spanning cluster first appears is called the critical point and denoted by p_c , meaning the occupation probability at the critical point. The figure (5.10) shows the graph of the spanning probability, $W(p, L)$, versus the occupation probability p for different interactions (L_1, L_2) for different lengths. We have found that p_c is 0.5782, 0.5701 for L_1, L_2 respectively. From figure (5.4a) we know the p_c value for L_0 and it is 0.5927. Thus for long range interaction p_c is smaller than for short range interaction. The quantity $w(p, L)$ is called the spanning probability in a non periodic case and wrapping probability in a periodic case. The question is how do we find the wrapping probability, given that we have a list of p_c for different length. Note that for a certain length L , in each realization the p_c is not exact value, instead it is a range of values that contains the p_c . For example, say we have a lattice of length 200 and for that we will have different p_c at each realization. After an infinite number of experimentation we

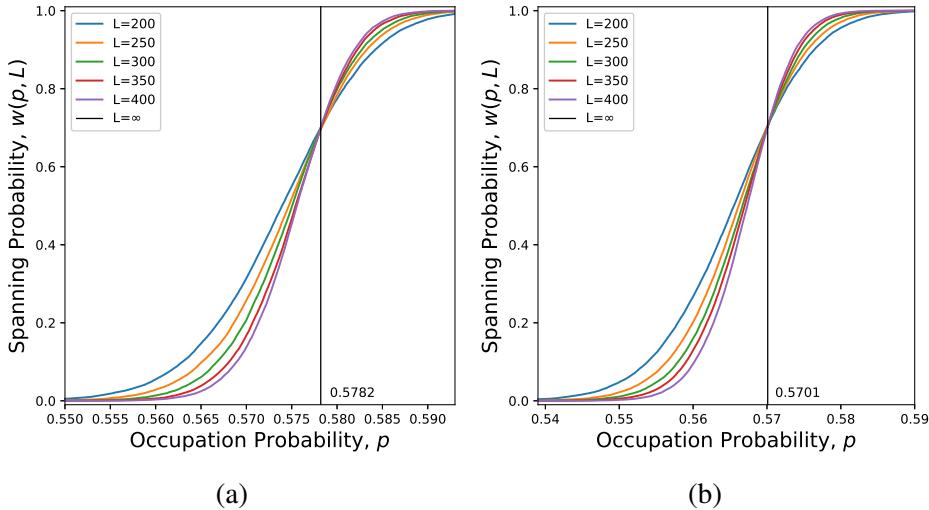


Fig. 5.10 Spanning probability $W(p, L)$ vs p for different lattice sizes using new definition of site percolation for (a) L_1 and (b) L_2 interaction. We find the threshold (critical point) which is the intersection of curves of different lattice sizes and we get 0.5782 and 0.5701 as p_c for (a) L_1 and (b) L_2 .

will have to take an average and that will give the exact value of p_c . But since it is practically impossible, we can find $p_{c_{avg}}$ for different lattice size then from the graph we can extrapolate the exact value of p_c for infinite lattice. Here $p_{c_{avg}}$ is calculated from a finite set of p_c for a certain length. This process is not good enough. Since it requires $p_{c_{avg}}$'s for a number of lattice size which is very costly to obtain. But from the data, list of p_c 's for different length, we can find the cumulative frequency distribution. It is astonishing that for all length the wrapping probability coincide at a specific point. This implies that if we could have an infinite system, the wrapping probability for that system would have gone through this same point. This means we have got our critical point, p_c , as the intersection of the $W(p, L)$ for different lengths.

5.2.2 Spanning Probability and finding $1/v$

From the figure (5.10) we can see that, as we increase the length of the lattice the wrapping probability $W(p, L)$ moves closer and closer to the critical point. And if we draw a horizontal line at a certain height (close to the bottom), say $y = 0.15$, and find the intersection of this line with $W(p, L)$ for each length and note the p and if we plot $\log(L)$ vs $\log(p - p_c)$ we get the slope $1/v$. which is shown in the inset of the figure (5.12).

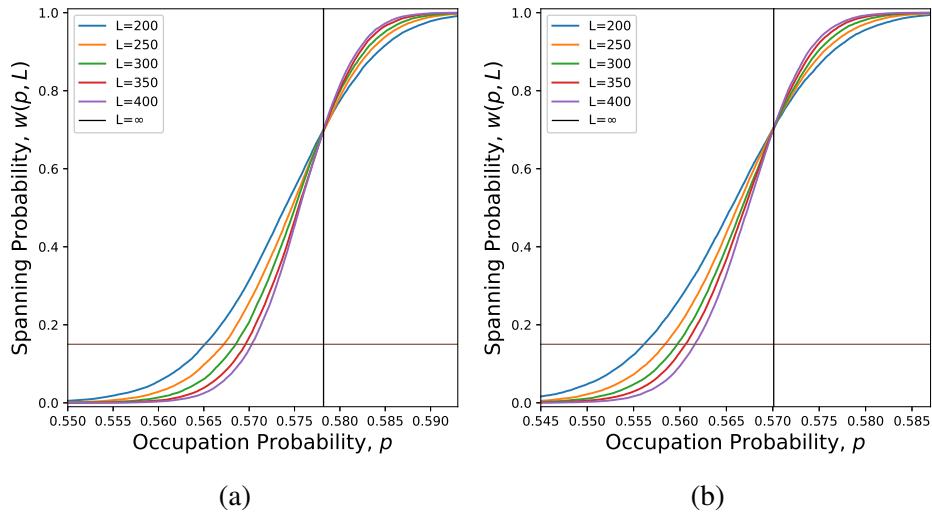


Fig. 5.11 A horizontal line is plotted at height $h \sim 1.5$ which at the bottom of the graph. We measure the distance from the vertical line (black) to the intersection of the curves for different lattice size, L and call them $(p - p_c)$ where p_c is the critical point (black line). The plot of $\log(L)$ vs $\log(p - p_c)$ gives us the exponent that scales the x -values of these curves.

If we now use the finite size scaling (FSS) hypothesis

$$W = (p - p_c)L^{1/\nu} \quad (5.6)$$

and plot W vs $(p - p_c)L^{1/\nu}$ we find excellent data collapse and it is shown in figure (5.11) we get a very good data collapse for L_1, L_2 and got $1/\nu$ as $0.736, 0.721$ respectively which is shown in figure 5.12. From the discussion of chapter (2) we know that the data collapse means that a system is self-similar, that is for any size of lattice L we will get the exact same collapse if we use the exponent $1/\nu$ obtained here for L_1 and L_2 .

5.2.3 Entropy, Specific Heat and finding α

For any phase transition model the entropy is crucial since it determines the type of transition. In percolation theory we use Shannon Entropy [121]. Using the definition from section (4.6.3) we get the figure (5.13).

Now we attempt to find the specific heat. Since the specific heat $C(p, L)$ is defined in section (4.6.4), we simply use the relation (4.17) to obtain the specific heat for percolation in square lattice. But we get a noisy data and we call it micro-canonical. We apply convolution

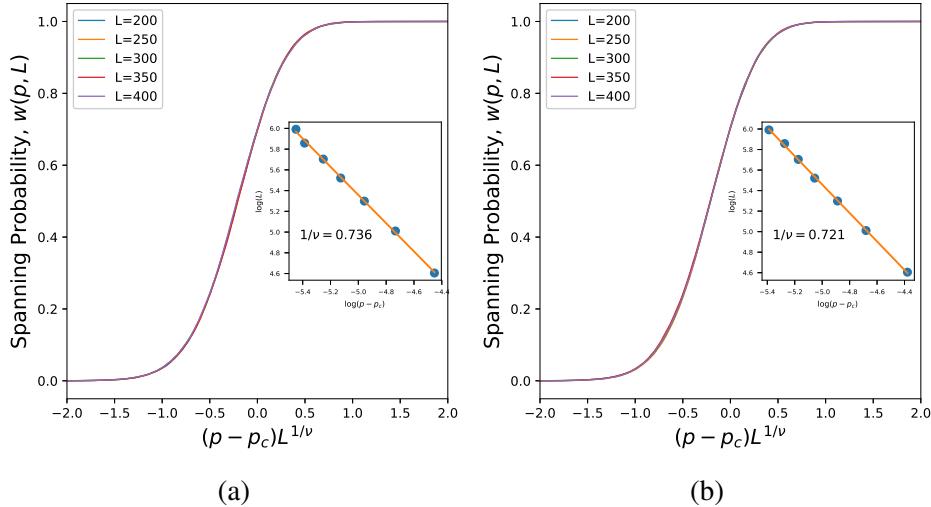


Fig. 5.12 We plot dimensionless quantities W vs $(p - p_c)L^{1/\nu}$ using value of $1/\nu = 0.736, 0.721$ respectively for (a) L_1 and (b) L_2 for which we find excellent data-collapse. The values of $1/\nu$ is obtained from figure (5.11) by plotting $\log(L)$ vs $\log(p - p_c)$ which is shown in the inset of this graph.

formula to get specific heat for a canonical ensemble. The process of applying convolution is described in appendix (B). After applying convolution we a smooth curve shown in figure (5.14).

From specific heat we can find the exponent α . To do this first we need to scale the x -values of the specific heat data using the exponent $1/\nu$ obtained from (5.2.2) and get the graph as in figure (5.15). From this graph we will get the height of each line and call it C_h . Since each line corresponds to a specific length L we can plot $\log(C_h)$ versus $\log(L)$ and the absolute value of the graph will give α/ν and from that we can find the exponent α simply by dividing α/ν by $1/\nu$. We get α values 0.911, 0.919 for L_1, L_2 correspondingly. and using this value we can apply FSS hypothesis to get data collapse. If we plot $CL^{-\alpha/\nu}$ vs $(p - p_c)L^{1/\nu}$ we get perfect data collapse for L_1, L_2 and it is shown in figure (5.16)

5.2.4 Order Parameter and finding β

Order parameter, also known as the percolation strength, is ,along with entropy, an important quantity in the study of phase transition. It is denoted as $P(p, L)$. Using the definition (4.21) we obtain the order parameter for our system and it is shown in the figure (5.17). Since using spanning cluster and the largest cluster gives the same exponent, it really does not matter

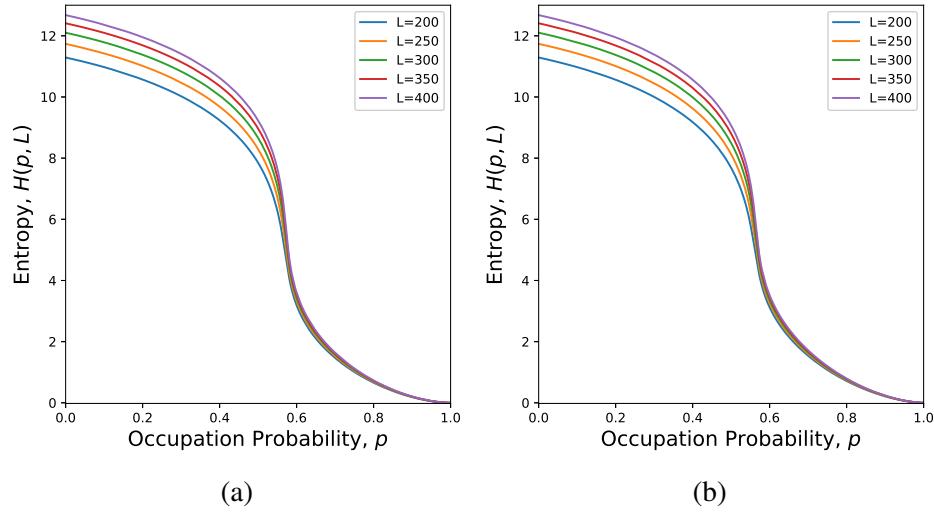


Fig. 5.13 Entropy, $H(p,L)$ vs Occupation Probability, p for (a) L_1 and (b) L_2 interaction in square lattice whose p_c values are 0.5782 and 0.5701 respectively

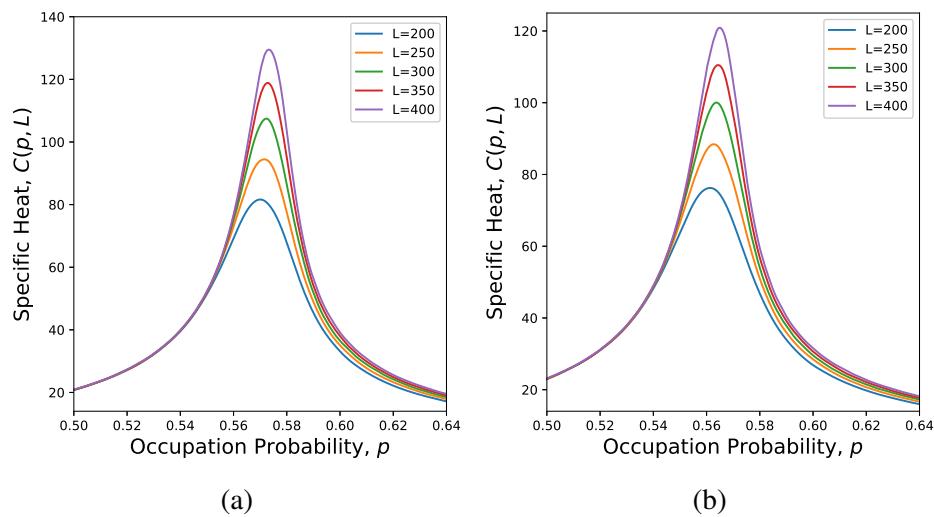


Fig. 5.14 Specific Heat, $C(p,L)$ vs Occupation Probability, p for (a) L_1 and (b) L_2 interaction.

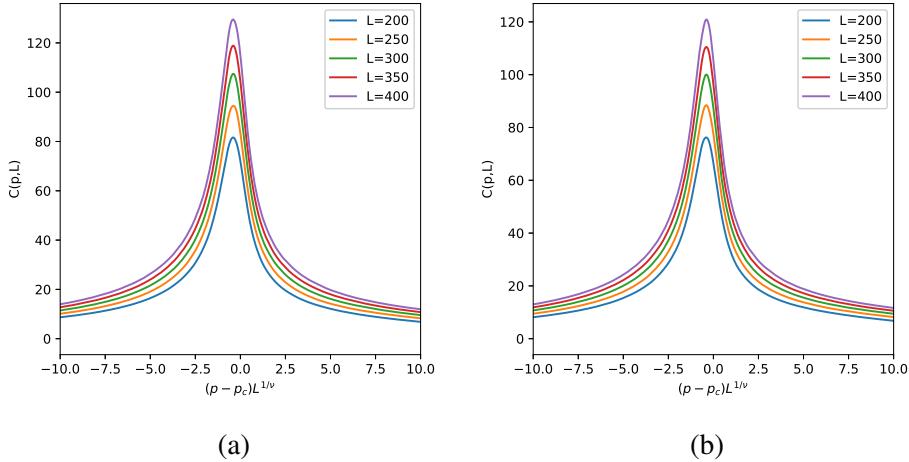


Fig. 5.15 We plot $C(p, L)$ vs $(p - p_c)L^{1/\nu}$ using values of $1/\nu$ obtained from section (5.2.2) for (a) L_1 and (b) L_2 . We then measure height of the curves and call it C_h . Then plotting $\log(C_h)$ vs $\log(L)$ gives us the exponent α/ν which is shown in the inset of figure (5.16)

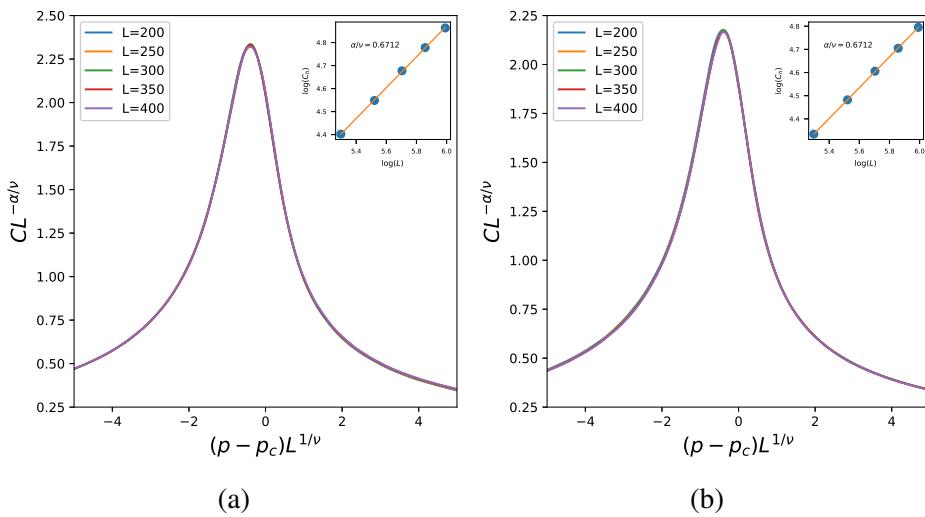


Fig. 5.16 Plots of dimensionless quantities $CL^{-\alpha/v}$ vs $(p - p_c)L^{1/v}$ for different sizes of square lattice for (a) L_1 and (b) L_2 interaction. We know the values of $1/v$ for corresponding interaction from section (5.2.2). We find excellent data collapse with $\alpha/v = 0.6712, 0.6631$ for (a) L_1 and (b) L_2 interaction respectively. Values of α/v is obtained from the graph $\log(C_h)$ vs $\log(L)$ which is shown in the inset and C_h is known to us from figure (5.15)

which one we use. But in our case there is a boundary of the system, which we define as periodic. Hence using spanning cluster is appropriate. Using the exponent $1/\nu$ obtained

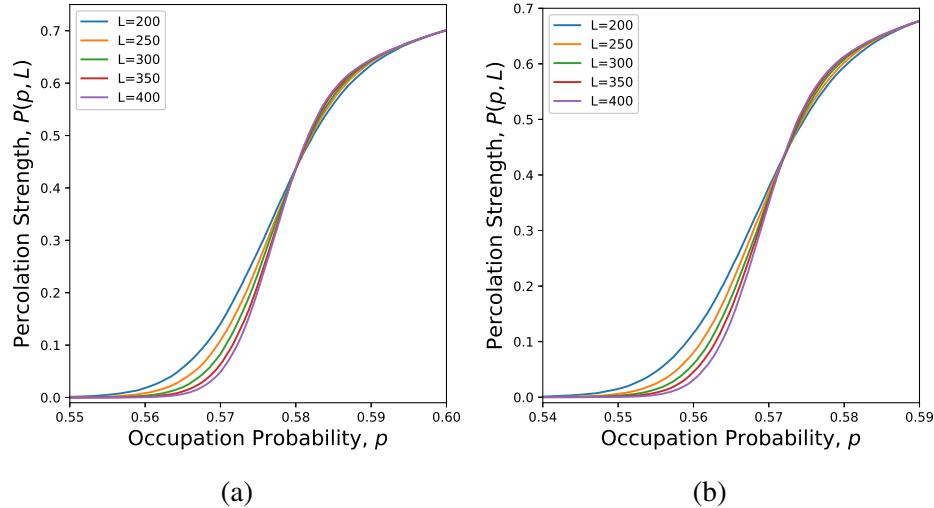


Fig. 5.17 Order Parameter, $P(p,L)$ vs Occupation Probability, p for (a) L_1 and (b) L_2

in section (5.2.2) we scale the x -values as $(p - p_c)L^{1/\nu}$ and get the following figure (5.18). Then in figure (5.18) we draw a vertical line where there are several horizontal lines. We measure the height of the lines and call it P_h and after plotting $\log(P_h)$ vs $\log(L)$ (inset of figure (5.19))we get the exponent β/ν from it's slope and obtain exponent β by dividing β/ν by $1/\nu$. Using the FSS hypothesis (2.4.2) we plot $PL^{\beta/\nu}$ versus $(p - p_c)L^{1/\nu}$ and get a good data collapse which is shown in figure (5.19).

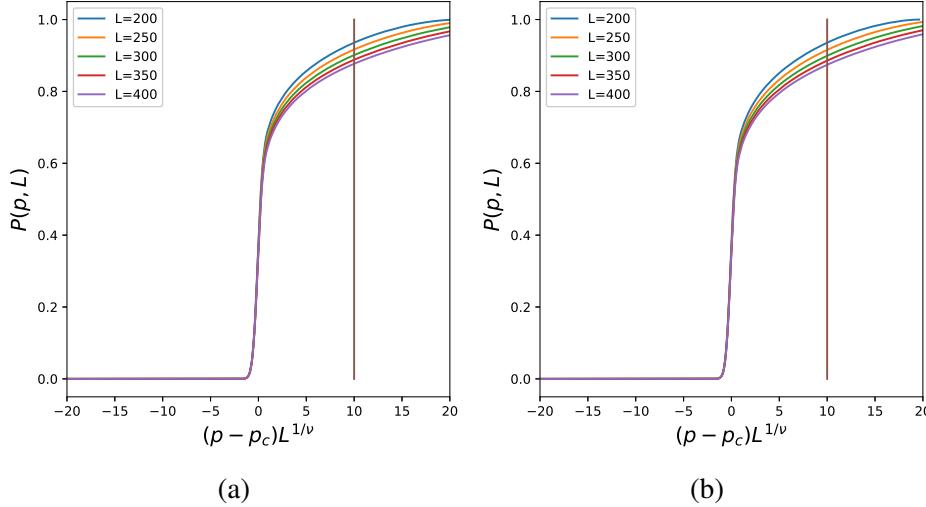


Fig. 5.18 Order Parameter, $P(p, L)$ vs dimensionless quantity $(p - p_c)L^{1/v}$ for (a) L_1 and (b) L_2 interactions. The values of $1/\nu$ is obtained from section (5.2.2). We draw a vertical line near the critical point and measure the height of the intersection of the curves of P with the vertical line and call it P_h . The plot of $\log(P_h)$ vs $\log(L)$ gives us the exponent γ/ν which is shown in the inset of the figure (5.19)

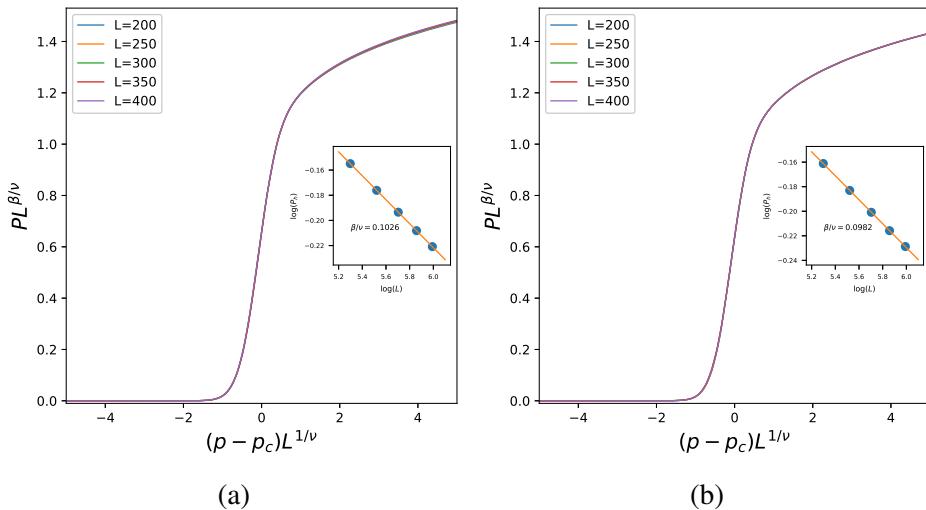


Fig. 5.19 We plot $P(p, L)L^{\beta/\nu}$ versus $(p - p_c)L^{1/v}$ using the values of $1/\nu$ from section (5.2.2). And the value of the exponent β/ν obtained from the plot in the inset of this graph. To do this we needed values of P_h which is obtained from figure (5.18). An excellent data collapse is obtained using the exponents $\beta/\nu = 0.1026, 0.0982$ for (a) L_1 and (b) L_2 respectively.

5.2.5 Susceptibility and finding γ

Susceptibility is defined as the derivative of the order parameter $P(p, L)$ with respect to the control parameter p , i.e., $\chi = \frac{dP}{dp}$. Using this definition we obtain the graph of susceptibility (5.20).

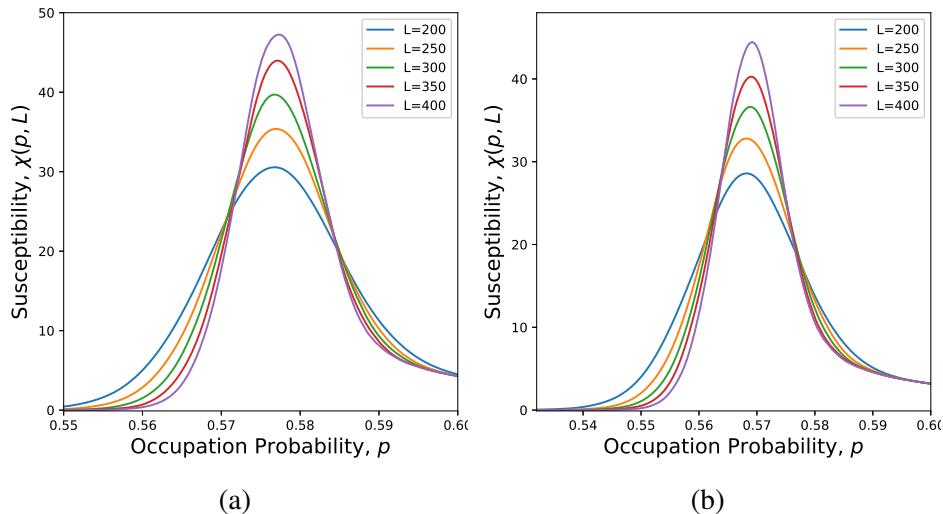


Fig. 5.20 Plots of susceptibility $\chi(p)$ as a function of p in square lattice of different sizes for (a) L_1 and (b) L_2 interaction.

And if we scale the x values and plot χ vs $(p - p_c)L^{1/\nu}$ we get all the peak point aligned (figure (5.21)). Note that the value of $1/\nu$ is known from section (5.2.2). Then we take the reading of the height of each line and call it χ_h . Since each line represents a different lattice size, plotting $\log(\chi_h)$ vs $\log(L)$ gives the slope γ/ν .

And using the FSS hypothesis we plot $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ and obtain a perfect data collapse. It is shown in figure (5.22). We obtain the values of γ to be 0.8542, 0.882.

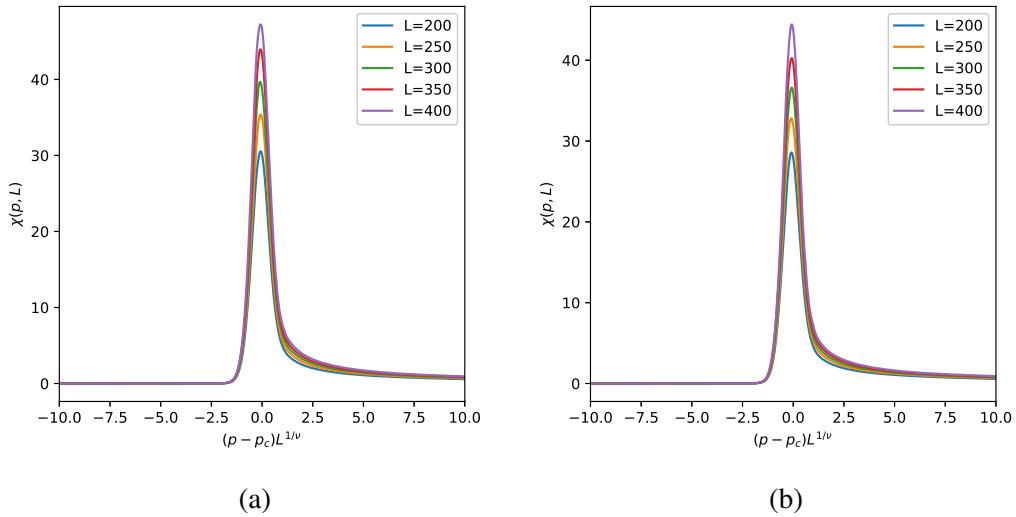


Fig. 5.21 We plot $\chi(p, L)$ vs $(p - p_c)L^{1/\nu}$ using the values of $1/\nu$ obtained from section (5.2.2). Then we measure the height of the curves and call them χ_h and plotting $\log(\chi_h)$ vs $\log(L)$ gives us the exponent γ/ν which is shown in the inset of figure (5.22).

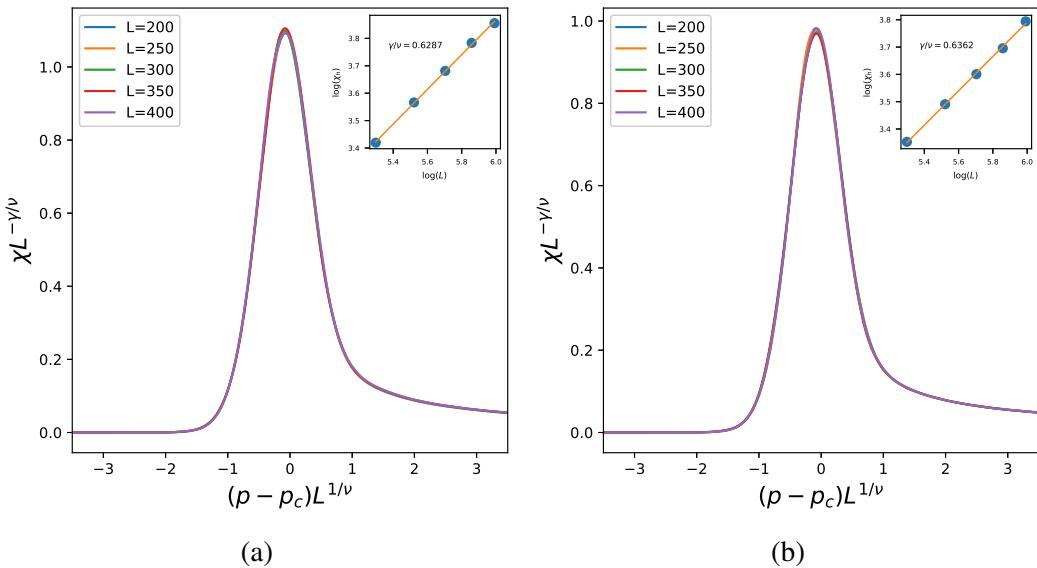


Fig. 5.22 Plots of dimension less quantities $\chi L^{\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ for different sizes of square lattice for (a) L_1 and (b) L_2 interaction. We know the values of $1/\nu$ for corresponding interaction from (5.2.2). We find excellent data collapse with $\gamma/\nu = 0.6287, 0.6362$ for (a) L_1 and (b) L_2 interaction respectively. Values of γ/ν is obtained from the graph $\log(\chi_h)$ vs $\log(L)$ which is shown in the inset and χ_h is known to us from figure (5.21)

5.2.6 Fractal Dimension

At critical point the square lattice shows the property of a fractal [49] (4.6.7). We use the relation

$$S \sim L^{d_f} \quad (5.7)$$

taking log we get

$$\log(S) = d_f \log(L) \quad (5.8)$$

Here S is the average size of the spanning cluster at critical point. Using this we get the figure (??). And we obtain fractal dimension d_f for L_0, L_1, L_2 which is listed in (??). Fractal

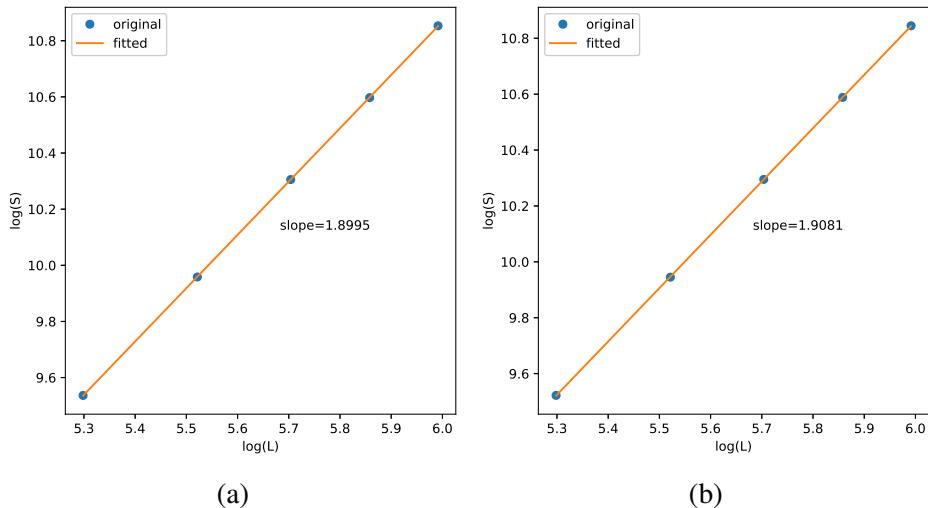


Fig. 5.23 We plot $\log(S)$ vs $\log(L)$ where S is the size of the spanning cluster and L is the length of the lattice. We obtain the slope 1.8995 and 1.9081 for (a) L_1 and (b) L_2 respectively which are the fractal dimensions of the system for L_1 and L_2 interactions respectively.

dimension gives us the information about the size of the spanning(wrapper) cluster. If the lattice size is known we can estimate the average size of the spanning cluster using d_f and (5.7).

5.2.7 Order-Disorder Transition

Phase transition is an order-disorder transition. There is a critical point which separates the two regions. Before the critical point the system is in disordered phase and after it is in ordered phase when we increase temperature in thermodynamics. Behavior of two phases

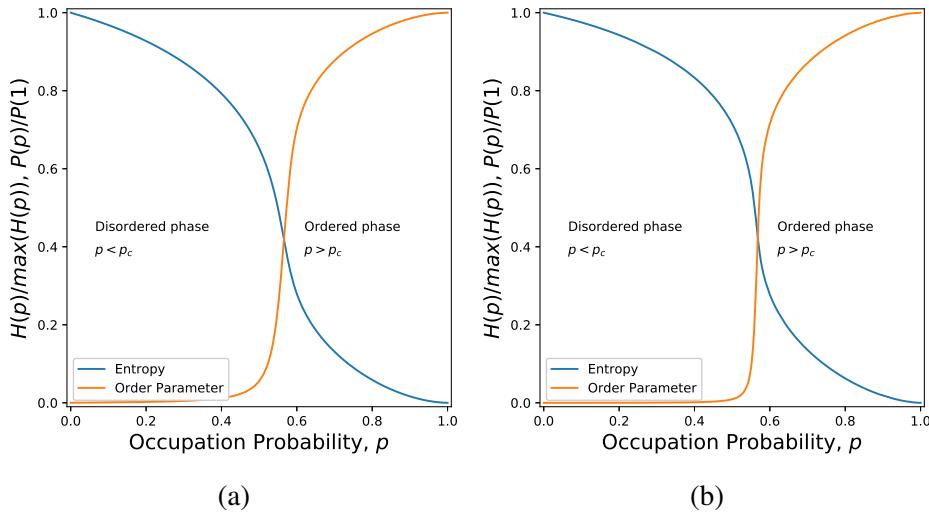


Fig. 5.24 We plot normalized entropy $H(p,L)/H(0,L)$ and normalized order parameter $P(p,L)/P(1,L)$ vs p in one graph to see the order disorder transition in square lattice for (a) L_1 (b) L_2 interaction. We had to normalize entropy to make order parameter and entropy comparable.

are completely different. It's astonishing how the behavior changes. In percolation theory, this order disorder transition is different than in thermodynamics.

Here disordered means uncertainty, since we are dealing with a system where probability is the control parameter (the occupation probability p). When p is minimum all clusters are disconnected and have size of unity. This means that we can to pick a cluster with probability $\frac{1}{2L^2}$, where L is the lattice size and $2L^2$ is the number of bonds in the lattice. That's why entropy is maximum and order parameter is minimum in this region. Now as we keep occupying the lattice clusters of different size arises, and at some point a miracle happens. It is the critical point where the transition occurs. A cluster appears for the first time which spans the entire lattice either horizontally or vertically. And in case of periodic condition the cluster wraps the lattice all the way around it. This cluster is called the spanning (wrapping) cluster in non-periodic (periodic) condition. The probability of picking this cluster at random is always larger than picking any other clusters. Thus system goes to the ordered state. And if we keep occupying the lattice at some point all cluster are joined to form one cluster. Thus picking this cluster at random has no uncertainty, meaning we have reached the entirely ordered phase. Here entropy is minimum and ordered parameter is maximum. A graph (5.24)

containing both entropy and order parameter can show this process. We have normalized the entropy (figure (5.13)) to match with the order parameter (figure (5.17)).

Chapter 6

Summary and Discussion

We have first discussed entropy for percolation. Note that percolation is a probabilistic model and hence Shannon entropy is the only hope if we want to measure entropy for percolation. To measure the Shannon entropy for percolation we have defined the cluster picking probability μ_i that a site is picked at random belongs to the labelled cluster i . It gives entropy which is consistent with the behaviour of the order parameter. Essentially entropy measures the degree of disorder while order parameter measures the extent of order. Thus, entropy and order parameter cannot be minimum or maximum at the same state since the system cannot be in most disordered and most ordered state at the same time. However, by measuring entropy and order parameter using existing definition for site percolation, we find that at $p = 0$ both order parameter and entropy equal to zero which is absurd. It demands immediate correction to the definition of entropy and we obliged. Note that in the bond percolation we occupy bond to connect sites and measure clusters by the number of sites. In analogy with that we redefine the site percolation as follows. We occupy sites to connect bonds which are assumed to exist already in the system and measure clusters in terms of the number of bonds. On the other hand, occupation probability in the bond (site) percolation is the fraction of bonds (sites) occupied in the system. With this new definition we have found the entropy behaves exactly in the same way as it does in the case of its bond counterpart. Thus the conflict that the system is in ordered and disordered at the same state is resolved.

The question that arises then is: Do we recover all the known results? To verify this we obtained all the necessary critical exponents with the new definition for site percolation. Earlier it was well-known that bond and site percolation belong to the same universality class

regardless of the nature of lattice but have the same dimension. We have confirmed that bond and redefined site percolation still belong to the same universality class. Note that scaling theory predicts that the various critical exponents cannot just assume values independently rather they are bound by some scaling and hyperscaling relations. One of the most interesting relations is the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$. Substituting our values of $\alpha = 0.906$, $\gamma = 0.8543$ and already known value of $\beta = 0.137$ we find $\alpha + 2\beta + \gamma = 2.0347$. We can thus conclude that the RI holds almost as equality but marginally greater than 2.

Then we have investigated percolation by random sequential ballistic deposition (RSBD) on a square lattice with interaction range upto second nearest neighbors. The critical points p_c and all the necessary critical exponents α, β, γ, v etc. are obtained numerically for each range of interactions. Like in its thermal counterpart, we find that the critical exponents of RSBD depend on the range of interactions and for a given range of interaction they obey the Rushbrooke inequality. We obtain the fractal dimension d_f that characterizes the spanning cluster at p_c . Our results suggest that the RSBD for each range of interaction belong to a new universality class which is in sharp contrast to earlier results of the only work that exist on RSBD.

We denote L_0, L_1, L_2 for expressing direct, first nearest neighbor and second nearest neighbor interaction respectively. Obviously L_0 denotes the regular kind of site percolation where we choose a site randomly with uniform probability and occupy it if it is empty else we skip the step. And L_1 is the class where we choose one of the four neighbor to occupy whenever we fail to do L_0 but only if the neighbor is empty else we skip the step. Finally in L_2 we choose the neighbor in the direction of the second neighbor, which was picked but was not empty, to occupy if it is empty else we skip the step. We have found that for L_1 and L_2 the exponents α, β, γ, v are consistent and they belong to a universality class respectively. Note that we can use new feature of L_1 only if the feature of L_0 is unavailable, i.e., the selected site is already occupied. Similarly we can use new feature of L_2 only if the feature of L_0 and L_1 is unavailable. Using this in mind we perform simulation and we obtain the critical exponents which agree with the laws of thermodynamics and the Rushbrooke inequality is satisfied in all cases.

6.1 Results

Here we list all the exponents found in our investigation of site percolation after redefining it and the RSBD model. Table (6.1) Lists all the critical values and exponents as we find them in our exponents. Note that we can get the exponent a , for example, from exponent a/v simply by dividing them by $1/v$ which is shown in table (6.2) where we also show that the Rushbrooke inequality is satisfied.

Interaction	p_c	$1/v$	α/v	β/v	γ/v
L_0	0.5927	0.75	0.6799	0.103	0.64071
L_1	0.5782	0.736	0.6712	0.1026	0.6287
L_2	0.5701	0.721	0.6631	0.0982	0.6362

Table 6.1 List of combined exponents

Interaction	α	β	γ	$\alpha + 2\beta + \gamma$
L_0	0.906	0.137	0.8543	2.0347
L_1	0.911	0.139	0.8542	2.044
L_2	0.919	0.136	0.882	2.07

Table 6.2 Exponents Satisfying Rushbrooke Inequality

Finally we list all the fractal dimensions, d_f , for different interactions in table (6.3).

Interaction	d_f
L_0 (standard)	91/48
L_0 (obtained)	1.8939
L_1	1.8994
L_2	1.9081

Table 6.3 Fractal dimensions for L_0, L_1, L_2 respectively.

Here we notice that the critical point decreases as we increase the range of interaction. But the fractal dimension increases. This is reasonable since by occupying nearest and second nearest neighbor we are increasing the chance of any individual cluster to grow faster. This is the reason for the p_c value to decrease. But it grows in area not in length average meaning when the spanning cluster appears it will contain more sites and bonds than in regular percolation which is evident from the fractal dimension d_f . All other exponents

changes a bit but their shape is not different. That's why change is not visible to the naked eye and it requires a thorough investigation.

6.2 Further Research

The idea of RSBD model can be applied to many other lattice structures. Notice that in square lattice we only have four neighbors for a site but in other structures of lattice we may have more or less than four neighbors for one site, e.g. honeycomb lattice, triangular lattice. Here we have only considered interaction up to second nearest neighbor which can be extended to an arbitrary range but it will only be effective if we take the lattice size to be large. Instead of single layer formation we can go for multi-layer formation since in real world if we drop particles (for example sand or grain) in a confined space then it will create multiple layer form. Controlling the velocity parameter at which the particle moves to a certain direction can also be an interesting thing to do. We can try to involve particles of different sizes and apply the RSBD model which might give some interesting results.

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Appendix A

Percolation

A.1 Algorithm

The algorithm for RSBD is quite simple. Take a lattice of length L . It will contain L^2 frozen sites and $2L^2$ bond which are always present according to the new definition of site percolation. Then follow only option from below:

L0 pick a site randomly and then occupy it if the site is unoccupied and continue this process .

L1 pick a site randomly and then occupy it if the site is unoccupied and if it is already occupied choose one of the four neighbors to occupy. If the neighbors are unoccupied then occupy them else skip current iteration and continue this process.

L2 pick a site randomly and then occupy it if the site is unoccupied and if it is already occupied choose one of the four neighbors to occupy. If the neighbors are unoccupied then occupy them else choose the site next to the first selected neighbor to occupy. If the 2nd selected neighbor is unoccupied then occupy it else skip current iteration and continue this process.

Note that L1 includes L0 and L2 includes L1 and L0.

The UML diagram for the program is given in figure A.1.

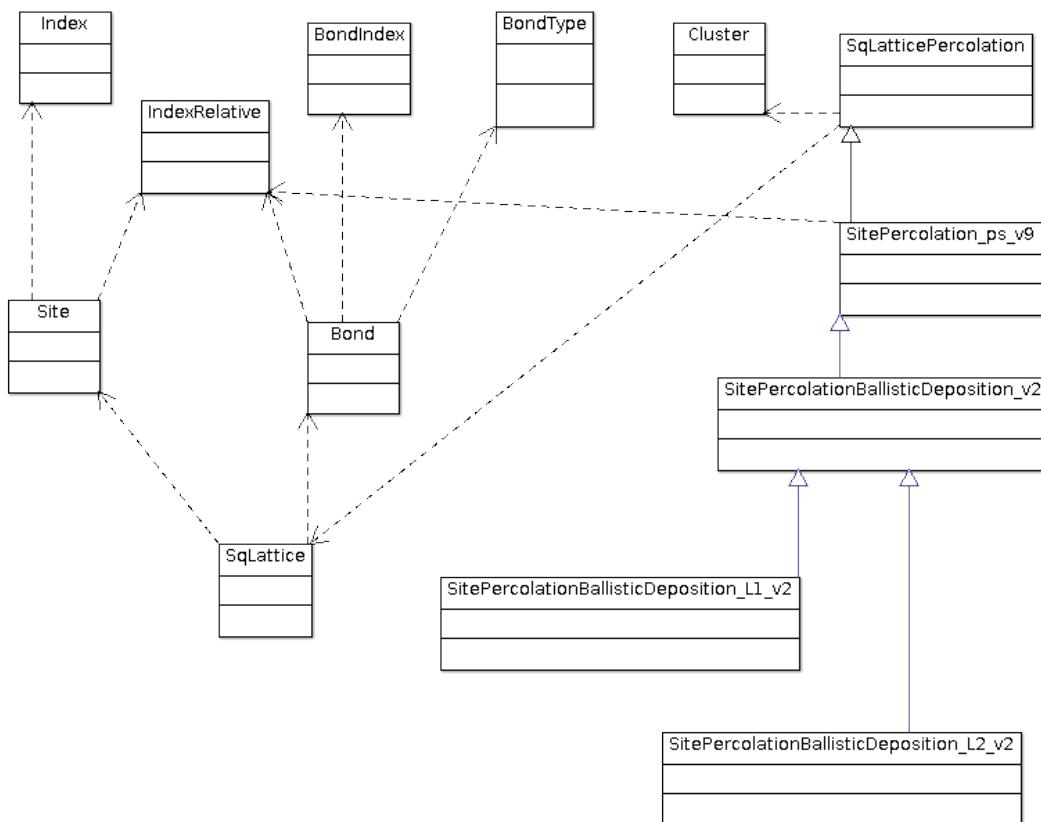


Fig. A.1 Schematic UML diagram for Site Percolation Ballistic Deposition program. This figure shows the dependencies and inheritance of the Classes and Structs in the program.

A.2 Code

Here only the declaration of certain classes are presented. All definitions are in the complete code and the link to the complete code is given in section (A.2.12).

A.2.1 Index

Here the notion of index of site and index of bond is defined. Site index has two element which determine row and column. Bond Index had three element describing bond type, row, column. Bond type can be horizontal or vertical.

the `src/index/index.h` file

```

1 struct Index{
2     value_type row_{ };
3     value_type column_{ };
4     ~Index() = default;
5     Index() = default;
6     Index(value_type x, value_type y) : row_{x}, column_{y} {}
7 };
8
9 class IndexRelative{
10 public:
11     int x_{ };
12     int y_{ };
13     ~IndexRelative() = default;
14     IndexRelative() = default;
15     IndexRelative(int x, int y) : x_{x}, y_{y} {}
16 };
17
18 struct BondIndex{
19     BondType bondType;
20     value_type row_;
21     value_type column_;
22     ~BondIndex() = default;
23     BondIndex() = default;
24     BondIndex(BondType hv, value_type row, value_type column)
25 : row_{row}, column_{column}

```

```

26 {
27 bondType = hv;
28 }
29 bool horizontal() const { return bondType == BondType::Horizontal; }
30 bool vertical() const { return bondType == BondType::Vertical; }
31 };
32
33 Index get_2nn_in_1nn_direction(Index center, Index nn_1, value_type
34 length);
35 std::vector<Index> get_2nn_s_in_1nn_s_direction(Index center, const std
36 ::vector<Index> &nn_1, value_type length);

```

A.2.2 Site

The site class contains all information about a site, e.g., if it is active or not and if it is then what is its group id or relative index.

The **src/lattice/site.h** file

```

1 struct Site{
2     bool _status{ false };
3     int _group_id{-1};
4     Index _id{};
5     IndexRelative _relative_index{0,0};
6     public:
7     ~Site() = default;
8     Site() = default;
9     Site(const Site&) = default;
10    Site(Site&&) = default;
11    Site& operator=(const Site&) = default;
12    Site& operator=(Site&&) = default;
13    Site(Index id, value_type length){
14        if(id.row_ >= length || id.column_ >= length){
15            std::cout << "out of range : line " << __LINE__ << std::endl;
16        }
17        _id.row_ = id.row_;
18        _id.column_ = id.column_;
19    }

```

```

20
21 bool isActive() const { return _status; }
22 void activate(){ _status = true; }
23 void deactivate() {
24     _relative_index = {0,0};
25     _group_id = -1;
26     _status = false;
27 }
28 Index ID() const { return _id; }
29
30 int     get_groupID() const { return _group_id; }
31 void    set_groupID(int g_id) { _group_id = g_id; }
32 std::stringstream getSite() const {
33     std::stringstream ss;
34     if(isActive())
35         ss << _id;
36     else
37         ss << "(*)";
38     return ss;
39 }
40
41 void relativeIndex(IndexRelative r){
42     _relative_index = r;
43 }
44 void relativeIndex(int x, int y){
45     _relative_index = {x,y};
46 }
47 IndexRelative relativeIndex() const { return _relative_index; }
48 };
49 std::ostream& operator<<(std::ostream& os, const Site& site);
50 bool operator==(Site& site1, Site& site2);

```

A.2.3 Bond

The bond class contains all information about a bond, e.g., if it is active or not and if it is then what is its group id.

The **src/lattice/bond.h** file

```
1 struct Bond{
2     bool _status{ false };
3     value_type _length;
4     int _group_id{-1};
5     BondType bondType;
6     IndexRelative _relative_index{0,0};
7     Index _end1;
8     Index _end2;
9     BondIndex _id;
10
11 ~Bond() = default;
12 Bond() = default;
13 Bond(Index end1, Index end2, value_type length){
14     _end1.row_ = end1.row_;
15     _end1.column_ = end1.column_;
16     _end2.row_ = end2.row_;
17     _end2.column_ = end2.column_;
18     _length = length;
19     if(_end1.row_ == _end2.row_){
20         bondType = BondType::Horizontal;
21         if(_end1.column_ > _end2.column_){
22             if(_end1.column_ == _length-1 && _end2.column_ == 0){
23                 }
24             else {
25                 _end1.column_ = end2.column_;
26                 _end2.column_ = end1.column_;
27             }
28         }
29         else if(_end1.column_ < _end2.column_){
30             if(_end1.column_ == 0 && _end2.column_ == _length-1){
31                 _end1.column_ = end2.column_;
32                 _end2.column_ = end1.column_;
33             }
34         }
35     }
36     else if(_end1.column_ == _end2.column_){
37         bondType = BondType::Vertical;
38         if(_end1.row_ > _end2.row_){
```

```
39 if (_end1.row_ == _length - 1 && _end2.row_ == 0) {
40 }
41 else {
42     _end1.row_ = end2.row_;
43     _end2.row_ = end1.row_;
44 }
45 }
46 else if (_end1.row_ < _end2.row_) {
47     if (_end1.row_ == 0 && _end2.row_ == _length - 1) {
48         _end1.row_ = end2.row_;
49         _end2.row_ = end1.row_;
50     }
51 }
52 }
53 else {
54     std::cout << '(' << _end1.row_ << ',' << _end1.column_ << ')' << "<->"
55     << '(' << _end2.row_ << ',' << _end2.column_ << ')'
56     << " is not a valid bond : line " << __LINE__ << std::endl;
57 }
58 _id = BondIndex(bondType, _end1.row_, _end1.column_); // unsigned long
59 }
60
61 std::vector<Index> getSites() const { return {_end1, _end2}; }
62 Index id() const { return _end1; }
63 BondIndex ID() const { return _id; }
64 void activate() { _status = true; }
65 void deactivate() {
66     _relative_index = {0,0};
67     _group_id = -1;
68     _status = false;
69 }
70 bool isActive() const { return _status; }
71
72 int get_groupID() const { return _group_id; }
73 void set_groupID(int g_id) { _group_id = g_id; }
74
75 bool isHorizontal() const { return bondType == BondType::Horizontal; }
76 bool isVertical() const { return bondType == BondType::Vertical; }
```

```

77 void relativeIndex(IndexRelative r){
78     _relative_index = r;
79 }
80 void relativeIndex(int x, int y){
81     _relative_index = {x,y};
82 }
83 IndexRelative relativeIndex() const {return _relative_index;}
84 };

```

The **src/lattice/bond_type.cpp** file

```

1 enum class BondType{
2     Horizontal,
3     Vertical
4 };

```

A.2.4 Lattice

The lattice class consists of array of sites and bonds. This class contains information about lattice size. And contains functions to view the lattice differently in the console.

the **src/lattice/lattice.h** file

```

1 class SqLattice {
2     std::vector<std::vector<Site>> _sites; // holds all the sites
3     std::vector<std::vector<Bond>> _h_bonds; // holds all horizontal bonds
4     std::vector<std::vector<Bond>> _v_bonds; // holds all vertical bonds
5     bool _bond_resetting_flag=true; // so that we can reset all bonds
6     bool _site_resetting_flag=true; // and all sites
7     value_type _length{};
8 private:
9     void reset_sites();
10    void reset_bonds();
11 public:
12    ~SqLattice() = default;
13    SqLattice() = default;
14    SqLattice(SqLattice&) = default;
15    SqLattice(SqLattice&&) = default;
16    SqLattice& operator=(const SqLattice&) = default;
17    SqLattice& operator=(SqLattice&&) = default;

```

```

18 SqLattice( value_type length , bool activate_bonds , bool activate_sites ,
    bool bond_reset , bool site_reset );
19 void reset(bool reset_all=false);
20
21 void activate_site(Index index);
22 void activateBond(BondIndex bond);
23 void deactivate_site(Index index);
24 void deactivate_bond(Bond bond);
25 value_type length() const { return _length; }
26 Site& getSite(Index index);
27 Bond& getBond(BondIndex);
28 const Site& getSite(Index index) const ;
29 const Bond& getBond(BondIndex index) const ;
30 void setGroupID(Index index , int group_id);
31 void setGroupID(BondIndex index , int group_id);
32 const int getGroupID(Index index) const;
33 const int getGroupID(BondIndex index) const;
34
35 std :: vector<Index> get_neighbor_site_indices(Index site); // site
    neighbor of site
36 std :: vector<BondIndex> get_neighbor_bond_indices(BondIndex site); // bond
    neighbor of bond
37 std :: vector<Index> get_neighbor_indices(BondIndex bond); // two site
    neighbor of bond.
38 static std :: vector<Index> get_neighbor_site_indices(size_t length , Index
    site); // 4 site neighbor of site
39 static std :: vector<BondIndex> get_neighbor_bond_indices(size_t length ,
    BondIndex site); // 6 bond neighbor of bond
40 static std :: vector<Index> get_neighbor_indices(size_t length , BondIndex
    bond); // 2 site neighbor of bond.
41 };

```

A.2.5 Exception

Different types of exceptions.

The **src/exception/exception.h** file

```

1 struct Mismatch{

```

```
2     std :: string msg_;
3     size_t line_;
4     Mismatch( size_t line , std :: string msg="" )
5             :line_{line}, msg_{msg} {}
6
7     void what() const {
8         std :: cerr << msg_ << "\nId and index mismatch at line " << line_
9         << std :: endl;
10    }
11
12 struct InvalidIndex{
13     std :: string msg_;
14     InvalidIndex( std :: string msg) :msg_{msg} {}
15
16     void what() const {
17         std :: cerr << msg_ << std :: endl;
18     }
19 };
20
21 struct InvalidBond{
22     std :: string msg_;
23     InvalidBond( std :: string msg) :msg_{msg} {}
24
25     void what() const {
26         std :: cout << msg_ << std :: endl;
27     }
28 };
29
30 struct OccupiedNeighbor{
31     std :: string msg_;
32     OccupiedNeighbor( std :: string msg): msg_{msg} {}
33
34     void what() const {
35         std :: cout << msg_ << std :: endl;
36     }
37 };
38
```

```

39 struct InvalidNeighbor{
40     std::string msg_;
41     InvalidNeighbor(std::string msg) :msg_{msg} {}
42     void what() const {
43         std::cout << msg_ << std::endl;
44     }
45 };

```

A.2.6 Cluster

The cluster class contains all information about a cluster. Number of sites and bonds in a cluster and the id of the cluster is contained in a cluster.

The `src/percolation/cluster.h` file

```

1 class Cluster{
2     std::vector<BondIndex> _bond_index;
3     std::vector<Index> _site_index;
4     int _creation_time {-1};
5     int _id {-1};
6     public:
7
8     ~Cluster() = default;
9     Cluster() = default;
10    Cluster(Cluster&) = default;
11    Cluster(Cluster&&) = default;
12    Cluster& operator=(const Cluster&) = default;
13    Cluster& operator=(Cluster&&) = default;
14
15    explicit Cluster(int id){
16        _id = id; // may be modified in the program
17
18        _creation_time = id + 1; // only readable, not modifiable
19    }
20    void addSiteIndex(Index );
21    void addBondIndex(BondIndex );
22    Index lastAddedSite(){return _site_index.back();}
23    BondIndex lastAddedBond(){return _bond_index.back();}

```

```

24 void insert(const std::vector<BondIndex>& bonds);
25 void insert(const std::vector<Index>& sites);
26 void insert(Cluster& cluster);
27 void insert_v2(Cluster& cluster);
28 void insert_with_id_v2(Cluster& cluster, int id);
29
30 friend std::ostream& operator<<(std::ostream& os, const Cluster& cluster
   );
31 const std::vector<BondIndex>& getBondIndices() { return _bond_index
   ;}
32 const std::vector<Index>& getSiteIndices() { return _site_index
   ;}
33 const std::vector<BondIndex>& getBondIndices() const { return
   _bond_index; }
34 const std::vector<Index>& getSiteIndices() const { return
   _site_index; }
35 value_type numberOfBonds() const { return _bond_index.size(); }
36 value_type numberOfSites() const { return _site_index.size(); }
37 int get_ID() const { return _id; }
38 void set_ID(int id) { _id = id; }
39 int birthTime() const { return _creation_time; }
40 Index getRootSite() const { return _site_index[0]; }
41 BondIndex getRootBond() const { return _bond_index[0]; }
42 bool empty() const { return _bond_index.empty() && _site_index.empty(); }
43 void clear() { _bond_index.clear(); _site_index.clear(); }
44 };

```

A.2.7 Percolation

The *SqLatticePercolation* class contains generic operation that to performed for percolation on square lattice. It's subclass *SitePercolation_ps_v9* is the class when all required method for general site percolation with our definition is defined. And it's subclass *SitePercolationBallisticDeposition_v2* contains some method for ballistic deposition for L_1, L_2 which extends to two new subclass *SitePercolationBallisticDeposition_L1_v2* and *SitePercolationBallisticDeposition_L2_v2* with detailed method for ballistic deposition L_1 and L_2 respectively.

The src/percolation/percolation.h file

```
1 class SqLatticePercolation{
2     value_type _length;
3     value_type _max_number_of_bonds;
4     value_type _max_number_of_sites;
5     char type{'0'}; // percolation type. 's' -> site percolation. 'b' ->
6         bond percolation
7 protected:
8     SqLattice _lattice;
9     value_type _index_sequence_position {};
10    std :: vector<Cluster> _clusters;
11    double _occupation_probability {};
12    double _entropy {};
13    double _entropy_current {};
14    size_t _cluster_count {};
15    value_type _bonds_in_cluster_with_size_two_or_more {0};
16    bool _reached_critical = false;
17    value_type _total_relabeling {};
18    double time_relabel {};
19    value_type _number_of_occupied_sites {};
20    value_type _max_iteration_limit {};
21    std :: random_device _random_device;
22    std :: mt19937 _random_generator;
23    void set_type(char t){type = t;}
24 public:
25    static constexpr const char* signature = "SqLatticePercolation";
26    virtual ~SqLatticePercolation() = default;
27    SqLatticePercolation(value_type length);
28    void reset();
29    bool occupy();
30    value_type length() const { return _length; }
31    value_type maxSites() const { return _max_number_of_sites; }
32    value_type maxBonds() const { return _max_number_of_bonds; }
33
34    virtual double occupationProbability() const { return
35        _occupation_probability; }
```

```
35 virtual double entropy() { return _entropy_current; }
36 double entropy_by_site(); // for future convenience. // the shannon
37     entropy. the full calculations. time consuming
38 double entropy_by_bond(); // for future convenience. // the shannon
39     entropy. the full calculations. time consuming
40 size_t number_of_cluster() const {return _cluster_count;}
41
42
43 void get_cluster_info(
44 std::vector<value_type> &site ,
45 std::vector<value_type> &bond
46 );
47
48
49 char get_type() const {return type;} // get percolation type
50 virtual value_type maxIterationLimit() {return _max_iteration_limit;};
51
52
53 double get_relabeling_time() const {return time_relabel;}
54 value_type relabeling_count() const {return _total_relabeling;}
55 };
56
57 /**
58 * Site Percolation by Placing Sites
59 * version 9
60 */
61 class SitePercolation_ps_v9 : public SqLatticePercolation{
62 protected:
63     bool _periodicity{false};
64     value_type min_index; // minimum index = 0
65     value_type max_index; // maximum index = length - 1
66
67     // index sequence
68     std::vector<Index> index_sequence;
69     std::vector<value_type> randomized_index;
70     int _cluster_id {};
71     value_type _index_last_modified_cluster {};
72     value_type _number_of_bonds_in_the_largest_cluster {};
73     value_type _number_of_sites_in_the_largest_cluster {};
```

```
71 Index _last_placed_site;      // keeps track of last placed site
72
73 std::vector<Index> _top_edge, _bottom_edge, _left_edge, _right_edge;
74 std::vector<Index> _spanning_sites;
75 std::vector<Index> _wrapping_sites;
76 std::vector<value_type> number_of_sites_to_span;
77 std::vector<value_type> number_of_bonds_to_span;
78 value_type _total_relabeling {};
79 void relabel_sites(const std::vector<Index> &sites, int id_a, int
80 delta_x_ab, int delta_y_ab);
81 double time_relabel {};
82 public:
83 static constexpr const char* signature = "SitePercolation_ps_v8";
84
85 ~SitePercolation_ps_v9() = default;
86 SitePercolation_ps_v9() = default;
87 SitePercolation_ps_v9(SitePercolation_ps_v9 &) = default;
88 SitePercolation_ps_v9(SitePercolation_ps_v9 &&) = default;
89 explicit SitePercolation_ps_v9(value_type length, bool periodicity=true)
90 ;
91
92 SitePercolation_ps_v9& operator=(SitePercolation_ps_v9 &) = default;
93 double get_relabeling_time() {return time_relabel;}
94 value_type relabeling_count() const {return _total_relabeling;}
95 virtual void reset();
96 bool periodicity() const {return _periodicity;}
97 std::string getSignature();
98 void add_entropy_for_bond(value_type index);
99 void subtract_entropy_for_bond(const std::set<value_type> &
100 found_index_set, int base=-1);
101 virtual bool occupy();
102 value_type placeSite_weighted(Index site); // uses weighted relabeling
103                                     by first identifying the largest cluster
103 value_type placeSite_weighted(Index site,
104 std::vector<Index>& neighbor_sites,
105 std::vector<BondIndex>& neighbor_bonds);
106 Index selectSite(); // selecting site
```

```

104 void connection_v2(Index site , std :: vector<Index> &site_neighbor , std ::  

105   vector<BondIndex> &bond_neighbor);  

106 void relabel_sites_v5(Index root_a , const Cluster& clstr_b); // relative  

107   index is set accordingly  

108 double numberOfOccupiedSite() const { return _number_of_occupied_sites; }  

109 double occupationProbability() const { return double(  

110   _number_of_occupied_sites)/maxSites(); }  

111 double entropy(); // the shannon entropy  

112 value_type numberOfBondsInTheLargestCluster_v2();  

113 value_type numberOfSitesInTheLargestCluster();  

114 value_type numberOfSitesInTheSpanningClusters_v2();  

115 value_type numberOfBondsInTheSpanningClusters_v2();  

116 value_type numberOfSitesInTheWrappingClusters();  

117 value_type numberOfBondsInTheWrappingClusters();  

118 bool detectSpanning_v6(const Index& site);  

119 bool check_if_id_matches(Index site , const std :: vector<Index> &edge);  

120 bool detectWrapping();  

121 void track_numberOfBondsInLargestCluster();  

122 void track_numberOfSitesInLargestCluster();  

123 Index lastPlacedSite() const { return _last_placed_site; }  

124 void spanningIndices() const;  

125 void wrappingIndices() const;  

126 void writeVisualLatticeData(const std :: string& filename , bool  

127   only_spanning=true);  

128 protected:  

129 void initialize();  

130 void initialize_index_sequence();  

131 void randomize_v2(); // better random number generator  

132  

133 int find_cluster_index_for_placing_new_bonds(const std :: vector<Index> &  

134   neighbors , std :: set<value_type> &found_indices);  

135  

136 value_type manage_clusters(  

137   const std :: set<value_type> &found_index_set ,  

138   std :: vector<BondIndex> &hv_bonds ,  

139   Index &site ,  

140   int base_id // since id and index is same  

141 );

```

```
137 public :
138     IndexRelative getRelativeIndex(Index root, Index site_new);
139 };
140
141
142 class SitePercolationBallisticDeposition_v2 : public
143     SitePercolation_ps_v9 {
144 protected:
145     std::vector<value_type> indices;
146     std::vector<value_type> indices_tmp;
147 public:
148     static constexpr const char* signature =
149         "SitePercolation_BallisticDeposition_v2";
150     virtual ~SitePercolationBallisticDeposition_v2() {
151         indices.clear();
152         indices_tmp.clear();
153     };
154     SitePercolationBallisticDeposition_v2(value_type length, bool
155         periodicity);
156     virtual bool occupy();
157
158     Index select_site(std::vector<Index> &sites, std::vector<BondIndex> &
159         bonds);
160     Index select_site_up_to_1nn(std::vector<Index> &sites, std::vector<
161         BondIndex> &bonds);
162     Index select_site_up_to_2nn(std::vector<Index> &sites, std::vector<
163         BondIndex> &bonds);
164
165     void reset();
166     void initialize_indices();
167
168     virtual std::string getSignature() {
169         std::string s = "sq_lattice_site_percolation_ballistic_deposition_";
170         if (_periodicity)
171             s += "_periodic_";
172         else
173             s += "_non_periodic_";
174         return s;
```

```
169 }
170 value_type placeSite_1nn_v2();
171 value_type placeSite_2nn_v1();
172 };
173
174 class SitePercolationBallisticDeposition_L1_v2: public
175     SitePercolationBallisticDeposition_v2{
176 public:
177 ~SitePercolationBallisticDeposition_L1_v2() = default;
178 SitePercolationBallisticDeposition_L1_v2(value_type length, bool
179     periodicity)
180 : SitePercolationBallisticDeposition_v2(length, periodicity){}
181
182 bool occupy() {
183 if(_number_of_occupied_sites == maxSites()){
184 return false;
185 }
186 try {
187 value_type v = placeSite_1nn_v2();
188 _occupation_probability = occupationProbability();
189 return v != ULONG_MAX;
190 } catch (OccupiedNeighbor& on){
191 return false;
192 }
193
194 std::string getSignature() {
195 std::string s = "sq_lattice_site_percolation_ballistic_deposition_L1";
196 if(_periodicity)
197 s += "_periodic_";
198 else
199 s += "_non_periodic_";
200
201 return s;
202 }
203
204 class SitePercolationBallisticDeposition_L2_v2: public
205     SitePercolationBallisticDeposition_v2 {
```

```

204 public :
205 ~SitePercolationBallisticDeposition_L2_v2() = default;
206 SitePercolationBallisticDeposition_L2_v2( value_type length , bool
207     periodicity )
208 : SitePercolationBallisticDeposition_v2( length , periodicity ){}
209
210 bool occupy() {
211 if (_number_of_occupied_sites == maxSites()){
212     return false;
213 }
214 try {
215     value_type v = placeSite_2nn_v1();
216     _occupation_probability = occupationProbability();
217     return v != ULONG_MAX;
218 } catch ( OccupiedNeighbor& on){
219     on.what();
220     return false;
221 }
222 std :: string getSignature() {
223     std :: string s = "sq_lattice_site_percolation_ballistic_deposition_L2 ";
224     if (_periodicity)
225         s += "_periodic_";
226     else
227         s += "_non_periodic_";
228     return s;
229 }
230 };

```

The src/percolation/percolation.cpp file

```

1 SqLatticePercolation :: SqLatticePercolation( value_type length ) {
2     if ( length <= 2) {
3         /*
4         * Because if _length=2
5         * there are total of 4 distinct bond. But it should have been 8, i.e., (2
6             * _length * _length = 8)
6 */

```

```
7 cerr << "_length <= 2 does not satisfy _lattice properties for"
     percolation : line" << __LINE__ << endl;
8 exit(1);
9 }
10 _length = length;
11 value_type _length_squared = length * length;
12 _max_number_of_bonds = 2*_length_squared;
13 _max_number_of_sites = _length_squared;
14 _clusters = vector<Cluster>();
15
16 //    size_t seed = 0;
17 //    cerr << "automatic seeding is commented : line " << __LINE__ <<
     endl;
18 auto seed = _random_device();
19 _random_generator.seed(seed); // seeding
20 cout << "seeding with " << seed << endl;
21 }
22
23
24 void
25 SqLatticePercolation::get_cluster_info(
26 vector<value_type> &site ,
27 vector<value_type> &bond
28 ) {
29 value_type total_site {}, total_bond {};
30 site.clear();
31 bond.clear();
32
33 unsigned long size = _clusters.size();
34 site.reserve(size);
35 bond.reserve(size);
36
37 value_type s, b;
38
39 for(value_type i{}; i < size; ++i){
40 if(_clusters[i].empty()){
41 //            cout << "Empty cluster : line " << endl;
42 continue;
```

```
43 }
44 s = _clusters[ i ].numberOfSites();
45 b = _clusters[ i ].numberOfBonds();
46 site.push_back(s);
47 bond.push_back(b);
48 total_site += s;
49 total_bond += b;
50 }
51 if( site.size() != bond.size() ){
52 cout << "Size mismatched : line " << __LINE__ << endl;
53 }
54 //    cout << "total bonds " << total_bond << endl;
55 //    cout << "total sites " << total_site << endl;
56 if(type == 's'){
57 for(value_type j{total_bond}; j < maxBonds(); ++j){
58 bond.push_back(1); // cluster of length 1
59 total_bond += 1;
60 }
61 }
62 if(type == 'b'){
63 for(value_type j{total_site}; j < maxSites(); ++j){
64 total_site += 1;
65 site.push_back(1); // cluster of length 1
66 }
67 }
68 }
69
70 void SqLatticePercolation::reset() {
71 _lattice.reset();
72 _clusters.clear();
73 _index_sequence_position = 0;
74
75 _occupation_probability = 0;
76 // entropy
77 _entropy=0;
78 _entropy_current=0;
79 _total_relabeling = 0;
80 time_relabel = 0;
```

```
81 _cluster_count = 0;
82 _reached_critical = false;
83 }
84
85
86 /**
87 * Entropy calculation is performed here. The fastest method possible.
88 * Cluster size is measured by site.
89 * @return current entropy of the lattice
90 */
91 double SqLatticePercolation::entropy_by_site() {
92 double H{}, mu ;
93
94 for(size_t i{}; i < _clusters.size(); ++i){
95 if(!_clusters[i].empty()){
96 mu = _clusters[i].numberOfSites() / double(_number_of_occupied_sites);
97 H += mu*log(mu);
98 }
99 }
100
101 return -H;
102 }
103
104 /**
105 * Entropy calculation is performed here. The fastest method possible.
106 * Cluster size is measured by site.
107 * @return current entropy of the lattice
108 */
109 double SqLatticePercolation::entropy_by_bond() {
110 double H{}, mu ;
111
112 for(size_t i{}; i < _clusters.size(); ++i){
113 if(!_clusters[i].empty()){
114 mu = _clusters[i].numberOfBonds() / double(maxBonds());
115 H += mu*log(mu);
116 }
117 }
```

```

119 double number_of_cluster_with_size_one = maxBonds() -
    _bonds_in_cluster_with_size_two_or_more;
120 //     cout << " _bonds_in_cluster_with_size_two_or_more " <<
    _bonds_in_cluster_with_size_two_or_more << " : line " << __LINE__ <<
    endl;
121 mu = 1.0/ double(maxBonds());
122 H += number_of_cluster_with_size_one * log(mu) * mu;
123
124 return -H;
125 }
```

A.2.8 Utilities

When generating data file we need to name our data file uniquely so that when all of the data files are in one location, no confusion occurs. A good way to do this is to add the time and data stamp at the end of each data file. Although data filename does share a common pattern.

A.2.9 Tests

A template function is required to run for *l0,l1,l2*. The template argument is the class name. The other two argument is the length and ensemble size we need for one file. The three template arguments are

1. SitePercolation_ps_v9
2. SitePercolationBallisticDeposition_L1_v2
3. SitePercolationBallisticDeposition_L1_v2

The **src/test/test_percolation.h** file

```

1 /**
2 * @tparam PType : Template type of percolation class
3 * @param argc   : argc from commandline
4 * @param argv   : argv from commandline
5 */
6 template<class PType>
```

```
7 void simulate_site_percolation_T(value_type length, value_type
8   ensemble_size) {
9
10  std::cout << "length " << length << " ensemble_size " << ensemble_size
11    << std::endl;
12
13  value_type length_squared = length*length;
14  value_type twice_length_squared = 2 * length_squared;
15
16  PType lattice_percolation(length, true);
17
18  std::ostringstream header_info;
19  header_info << "{"
20    << "\\" length \":\" << length
21    << ",\\" ensemble_size \":\" << ensemble_size
22    << ",\\" signature \":\" " << lattice_percolation.getSignature() << "\\" "
23    << "}" ;
24
25  std::string tm = getCurrentTime();
26
27  std::string filename_s = lattice_percolation.getSignature() + "
28    _cluster_by_site_" + std::to_string(length) + '_' + tm;
29  std::string filename_b = lattice_percolation.getSignature() + "
30    _cluster_by_bond_" + std::to_string(length) + '_' + tm;
31  std::string filename_critical = lattice_percolation.getSignature() + "
32    _critical_" + std::to_string(length) + '_' + tm;
33  std::string filename_entropy_order_parameter = lattice_percolation.
34    getSignature() + std::to_string(length) + '_' + tm;
35
36  std::ofstream fout_s(filename_s);
37 // JSON formated header
38  fout_s << '#' << header_info.str() << std::endl;
```

```

39 fout_s << "#each line is an independent realization" << std::endl;
40 fout_s << "#each line contains information about all clusters at
     critical point" << std::endl;
41 fout_s << "#cluster size is measured by number of sites in it" << std::
     endl;
42
43 std::ofstream fout_b(filename_b);
44 // JSON formated header
45 fout_b << '#' << header_info.str() << std::endl;
46 fout_b << "#each line is an independent realization" << std::endl;
47 fout_b << "#each line contains information about all clusters at
     critical point" << std::endl;
48 fout_b << "#cluster size is measured by number of bonds in it" << std::
     endl;
49
50 std::ofstream fout_critical(filename_critical);
51 fout_critical << '#' << header_info.str() << std::endl;
52 fout_critical << "#data at critical occupation probability or pc" << std
     ::endl;
53 fout_critical << "#<pc>,<sites in wrapping cluster>,<bonds in wrapping
     cluster>" << std::endl;
54
55 // simulation starts here
56 value_type counter {};
57 std::vector<double> entropy(lattice_percolation.maxIterationLimit());
58 std::vector<double> nob_wrapping(lattice_percolation.maxIterationLimit())
     ,
59 nob_largest(lattice_percolation.maxIterationLimit());
60
61 for(value_type i{} ; i != ensemble_size ; ++i){
62
63 lattice_percolation.reset();
64
65 bool successful = false;
66 auto t_start = std::chrono::system_clock::now();
67 counter = 0;
68 bool wrapping_written{false};
69 while (true){

```

```
70 successful = lattice_percolation.occupy();
71 if(successful) {
72 entropy[counter] += lattice_percolation.entropy();
73 nob_wrapping[counter] += lattice_percolation.
74     numberOfBondsInTheWrappingClusters();
75 nob_largest[counter] += lattice_percolation.
76     numberOfBondsInTheLargestCluster_v2();
77
78 if(!wrapping_written && lattice_percolation.detectWrapping()){
79     fout_critical << lattice_percolation.occupationProbability() << ","
80     << lattice_percolation.numberOfSitesInTheWrappingClusters() << ","
81     << lattice_percolation.numberOfBondsInTheWrappingClusters() << std::
82         endl;
83
84     std::vector<value_type> site , bond;
85
86     lattice_percolation.get_cluster_info(site , bond);
87
88     for(value_type j{}; j != site.size(); ++j){
89         fout_s << site[j] << ',' ;
90     }
91
92     for(value_type j{}; j != bond.size(); ++j){
93         fout_b << bond[j] << ',' ;
94     }
95
96     wrapping_written = true;
97
98
99     ++counter;
100 }
101 if(counter >= lattice_percolation.maxIterationLimit()){ //twice_length_squared is the number of bonds
102     break;
103 }
```

```
104 }
105
106 auto t_end = std::chrono::system_clock::now();
107 std::cout << "Iteration " << i << ". Elapsed time " << std::chrono::
108     duration<double>(t_end - t_start).count() << " sec" << std::endl;
109 }
110 fout_b.close();
111 fout_s.close();
112 fout_critical.close();
113
114
115 std::ofstream fout(filename_entropy_order_parameter);
116 fout << '#' << header_info.str() << std::endl;
117 fout << "#<p>,<H(p,L)>,<P1(p,L)>,<P2(p,L)>" << std::endl;
118 fout << "#p = occupation probability" << std::endl;
119 fout << "#H(p,L) = Entropy = sum( - u_i * log(u_i))" << std::endl;
120 fout << "#P1(p,L) = Order parameter = (number of bonds in largest
121     cluster) / (total number of bonds)" << std::endl;
122 fout << "#P2(p,L) = Order parameter = (number of bonds in spanning or
123     wrapping cluster) / (total number of bonds)" << std::endl;
124 fout << "#C(p,L) = Specific heat = -T dH/dT" << std::endl;
125 fout << "#X(p,L) = Susceptibility = dP/dp" << std::endl;
126 fout << "#u_i = (number of bonds in the i-th cluster) / (total number of
127     bonds)" << std::endl;
128 for(size_t i{}; i < lattice_percolation.maxIterationLimit(); ++i){
129     fout << (i+1) / double(lattice_percolation.maxIterationLimit()) << ",";
130     fout << entropy[i] / double(ensemble_size) << ",";
131     fout << nob_largest[i] / double(ensemble_size /* lattice_percolation.
132         maxBonds() */) << ",";
133     fout << nob_wrapping[i] / double(ensemble_size /* lattice_percolation.
134         maxBonds() */);
135     fout << std::endl;
136 }
137 fout.close();
138 }
```

A.2.10 Main

The main function receives 3 additional command line argument. First one is an integer $\{0, 1, 2\}$ which determine the range of interaction. Second one is the length of the lattice. For L_0 interaction use 0 and so on. And third one is the size of the ensemble. For example, 12005000 will run the program for $l = 1$, $L = 200$ for ensemble size of 5000.

The `run_in_main(int, char**)` function is the one where the `simulate_site_percolation_T<>(size_t, size_t)` executes for different classes.

The `src/main.cpp` file

```

1 #include <iostream>
2 #include <fstream>
3 #include <ctime>
4 #include <chrono>
5 #include <thread>
6 #include <mutex>
7 #include "lattice/lattice.h"
8 #include "percolation/percolation.h"
9 #include "util/time_tracking.h"
10 #include "util/printer.h"
11 #include "tests/test_percolation.h"
12 using namespace std;
13 /**
14 *   All the function that is run in main
15 */
16 void run_in_main(int argc, char** argv){
17 int l = atoi(argv[1]);
18 value_type length = atoi(argv[2]);
19 value_type ensemble_size = atoi(argv[3]);
20 if(l==1) {
21 cout << "Simulating site percolation for l=1" << endl;
22 simulate_site_percolation_T<SitePercolationBallisticDeposition_L1_v2>(
23     length, ensemble_size); // 2018.11.03
24 }
25 else if(l==2) {
26 cout << "Simulating site percolation for l=2" << endl;

```

```
26 simulate_site_percolation_T<SitePercolationBallisticDeposition_L2_v2>(
27     length , ensemble_size); // 2018.11.03
28 } else {
29     cout << "Simulating site percolation for l=0" << endl;
30     simulate_site_percolation_T<SitePercolation_ps_v9>(length , ensemble_size
31 );
32 }
33 /* **** */
34 * The main function
35 *****/
36 int main(int argc , char** argv) {
37     cout << "Running started at : " << currentTime() << endl;
38     cout << "Compiled on           : " << __DATE__ << "\t at " << __TIME__ <<
39         endl;
40     std::cout << "Percolation in a Square Lattice" << std::endl;
41     auto t_start = std::chrono::system_clock::now();
42     time_t seed = time(NULL);
43     srand(seed); // seeding
44     run_in_main(argc , argv);
45     auto t_end= std::chrono::system_clock::now();
46     std::chrono::duration<double> drtion = t_end - t_start;
47     std::time_t end_time = std::chrono::system_clock::to_time_t(t_end);
48     cout << "Program finished at " << std::ctime(&end_time) << endl;
49     std::cout << "Time elapsed " << getFormattedTime(drtion.count()) <<
50         std::endl;
51     return 0;
52 }
```

A.2.11 CMakeLists

All the header and source files are listed here and how the compiler should link them is generated by running cmake. <https://cmake.org/cmake-tutorial/>

A.2.12 complete code

Complete code for RSBD model on square lattice is available at

https://github.com/sha314/SqLattice_RSBD or use the git link to clone the repository

https://github.com/sha314/SqLattice_RSBD.git

Detailed version of the same program with other extensions are available at

<https://github.com/sha314/SqLatticePercolation> or the git link

<https://github.com/sha314/SqLatticePercolation.git>

Appendix B

Convolution

Say we want to measure an observable Q , for example, for a specific occupied number of sites(bonds) in site(bond) percolation. But doing this we ignore the fact that we would have chose to fix a probability p first and starting occupying the lattice sequentially then after we have had visited all the sites we would not have $p = n/(L^2)$ for site or $p = n/(2L^2)$ for bond percolation each time. Therefore it would lead to some error. We can solve this dilemma by the following process. The trick [68, 59] is to measure Q for fixed numbers of occupied sites (or bonds) n in the range of interest. Let us refer to the ensemble of states of a percolation system with exactly n occupied sites or bonds as a "microcanonical percolation ensemble," the number n playing the role of the energy in thermal statistical mechanics. The more normal case in which only the occupation probability p is fixed is then the "canonical ensemble" for the problem. (If one imagines the occupied sites or bonds as representing particles instead, then the two ensembles would be "canonical" and "grand canonical," respectively. Taking site percolation as an example, the probability of there being exactly n occupied sites on the lattice for a canonical percolation ensemble is given by the binomial distribution

$$B(N, n, p) = \binom{N}{n} p^n (1-p)^{N-n} \quad (\text{B.1})$$

The same expression applies for bond percolation, but with N replaced by M , the total number of bonds. Thus, if we can measure our observable within the microcanonical ensemble for all values of n , giving a set of measurements Q_n , then the value in the canonical ensemble

will be given by

$$Q(p) = \sum_{n=0}^N B(N, n, p) Q_n = \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} Q_n \quad (\text{B.2})$$

Thus we need only measure Q_n for all values of n . [98].

B.1 Algorithm

But using this formula to calculate $Q(p)$ is quite expensive since the number of sites(bonds) can be quite large direct evaluation of the binomial coefficients using factorials is not possible. We use alternative way to measure $Q(p)$, which is basically does the same thing but in an efficient way.

Instead, therefore, we recommend the following method of evaluation. The binomial distribution, Eq. (1), has its largest value for given N and p when $n = n_{max} = pN$. We arbitrarily set this value to 1. Now we calculate $B(N, n, p)$ iteratively for all other n from

$$B(N, n, p) = \begin{cases} B(N, n - 1, p) \frac{N-n+1}{n} \frac{p}{1-p} & \text{if } n > n_{max} \\ B(N, n + 1, p) \frac{n+1}{N-n} \frac{1-p}{p} & \text{if } n < n_{max} \end{cases}$$

Then we calculate the normalization coefficient $C = \sum_n B(N, n, p)$ and divide all the $B(N, n, p)$ by it, to correctly normalize the distribution [97, 98].

B.2 Code

In order to use convolution the following function can be used. It is very efficient and uses OpenMP for parallel run, meaning, all the cores of the processors performs the same task in a divide-and-conquer manner. This function takes an array as input and returns the convoluted version as output.

```

1  vector<double> convolution( vector<double>& data_in ) {
2      size_t N = data_in.size();
3      std::vector<double> _forward_factor(N);
4      std::vector<double> _backward_factor(N);

```

```
5   for (size_t i=0; i < N; ++i)
6   {
7     _forward_factor[i] = (double) (N - i + 1) / i;
8     _backward_factor[i] = (double) (i + 1) / (N - i);
9   }
10  vector<double> data_out(N);
11  long step = N / 1000;
12 #pragma omp parallel for schedule(dynamic)
13  for (long j=0; j < N; ++j) // start from j=1
14  {
15    double prob      = (double) j / N;
16    double factor    = 0;
17    double binom     = 0;
18    double prev      = 0;
19    double bn_tot    = 1; // normalization factor
20    double sum       = data_in[j];
21    // forward iteration part
22    factor = prob / (1-prob);
23    prev   = 1;
24    for (long i=j+1; i < N; ++i)
25    {
26      binom      = prev * _forward_factor[i] * factor;
27      bn_tot += binom;
28      sum       += data_in[i] * binom;
29      prev      = binom;
30    }
31    // backward iteration part
32    factor = (1-prob)/prob;
33    prev   = 1;
34    for (long i=j-1; i >= 0; --i)
35    {
36      binom      = prev * _backward_factor[i] * factor;
37      bn_tot += binom;
38      sum       += data_in[i] * binom;
39      prev      = binom;
40    }
41    // normalizing data
42    data_out[j] = sum / bn_tot;
```

```

43     cout << bn_tot << endl;
44 }
45 return data_out;
46 }
47

```

Complete code for convolution is available at <https://github.com/sha314/Convolution>.

The program linked above works using command line arguments. For example to perform convolution on a file "data.txt" which contains two columns out of which only second column needed to be convoluted use the following command.

<<<< HEAD

```
./convolute -f data.txt -a 0 -b 1
```

=====

```
\begin{lstlisting}[style=Instruction]
```

Usage:

```
convolution [-f <STRING>] [-a <INT>,<INT>,...[:<STRING>,<STRING>,...]]]
perform convolution based on provided options.
```

Options	Description
-a ,	columns that we want in the output file without
No default value .	
-b ,	columns that we want in the output file with p
No default value .	
-c ,	If provided the header and comment from the in
without modification to the output file . Header is the first line of the	
input file .	
-d	Delimiter to use . Default value is ' '.
-f	name of the input file that we want to convolu
-i	Info to write as comment in the output file
-o	name of the output file . If not provided the s
appended to the input file .	
-p , --precision	Floating point precision when writing in the d

-s Number of rows to skip from the input file.

-t to **test** the performance of the convolution p

--threads Explicitly specify number of thread to use. Defa

allowed by the system.

-h, --help display this **help** and **exit**

-v, --version output version information and **exit**

-w If provided input b data will be written to

The INT argument is an integer.

The STRING argument is a string of characters.

A line that begins with '#' is considered a commented line.

Exit status:

0 if OK,

1 if minor problems (e.g., cannot access subdirectory),

2 if serious trouble (e.g., cannot access command-line argument).

>>>>> 740a1659ba77aef0022f0942ef510ba892af4408

Appendix C

Finding Exponents

C.1 Algorithm

C.1.1 Specific Heat and Susceptibility

exponent for scaling the y -values

To find the best exponent for scaling the y -values of specific heat and susceptibility the following approach is pretty helpful.

Finding approximate value of the exponent

1. get the x and y values of the convoluted data for all lengths (L)
2. get the maximum value or the peak value of y as $y_{max} = \max(y)$ for each length
3. now plot $\log(y_{max})$ vs $\log(L)$
4. slope of this graph is the approximate value of the exponent

Finding the best exponent

Now that we know the approximate value of the exponent, ex_{approx} , we can find the best exponent in the following way

1. take a list of all the exponent in the range $E = [ex_{approx} - \varepsilon, ex_{approx} + \varepsilon]$ where ε is a small number (usually ~ 0.05)
2. for each value of the exponent a in the range above do the following

- (a) get the x and y values of the convoluted data for all lengths (L)
 - (b) scale the y value with the exponent and call it $y' = y * L^{-a}$
 - (c) get the maximum value or the peak value of y' as $y'_{max} = \max(y')$ for each length
 - (d) find the standard deviation of all the y'_{max} 's and call it std_a where the subscript denotes the current selected exponent
3. out of a number of selected exponent find the one with the minimum standard deviation and the exponent corresponding to this deviation is the best exponent denoted as a^* . Symbolically

$$a^* = \operatorname{argmin}_{a \in E} std_a \quad (\text{C.1})$$

exponent for scaling the x -values

Usually the exponent that scales the x -values is called $1/\nu$. The critical point is denoted as x_c . To find an estimate from the data that looks like the graph of specific heat or susceptibility, the following algorithm is very helpful

1. get the x and y values of the convoluted data for all lengths (L)
2. get the x value at a specific height, h , and call it x_h
3. plot a graph of $\log(|x_h - x_c|)$ vs $\log(L)$.
4. slope of this graph is the estimate for the exponent $1/\nu$

Now to find the exponent that best collapses the data is the main goal. To do this the following algorithm can be followed.

Finding the standard deviation of the points at height h after scaling x -values with an approximate value of the exponent ($1/\nu_{approx}$) that is obtained from the graph of $\log(|x_h - x_c|)$ vs $\log(L)$.

1. write a function that takes h , x_{scaler} , y_{scaler} , lr as argument where, h is the height at which we will be taking x -values, x_{scaler} is the exponent that scales the x -values, y_{scaler} is the exponent that scales the y -values and lr is the argument that tells if the left or right side of the critical point should be taken under consideration. call this function *find_x_deviation*

2. take $x' = (x - x_c)L^{x_{scaler}}$ and $y' = yL^{-y_{scaler}}$. Note that there is a minus sign used for scaling y values because the y_{max} increases as L increases in our present case which is observed when finding y_{scaler} previously.
3. at height h we draw a horizontal straight line and the intersection of this line with the curve gives corresponding x value at h . For each length L we obtain the x value and denote it with x_L .
4. after that we find the standard deviation of all x_L 's that we have found and this function returns the standard deviation
5. if lr is 0 then the left points of the critical point is considered and if lr is 1 then the right points of the critical point is considered for getting x_L 's.

Note that at a specific height there are two points on the left of the critical point and another is on the right. So if we find the exponent that best collapses the points on the left, it might not best collapse the points on the right C.1.

To resolve this problem we take following approach

1. take a range $ex = [(1/nu)_{approx} - \varepsilon, (1/nu)_{approx} + \varepsilon]$, where ε is usually ~ 0.05 .
2. for each value in this range find the standard deviation for left and right points of the critical point and call it d_{left} and d_{right} respectively
3. plot d_{left} vs ex and d_{right} vs ex on the same graph
4. the minima of line corresponding to d_{left} vs ex graph gives the exponent that collapses left points of the critical point at best.
5. the minima of line corresponding to d_{right} vs ex graph gives the exponent that collapses right points of the critical point at best.
6. the intersection of the graph is the value where both left and right points of the critical point fits better.

The figure C.1 gives the visual of the above process.

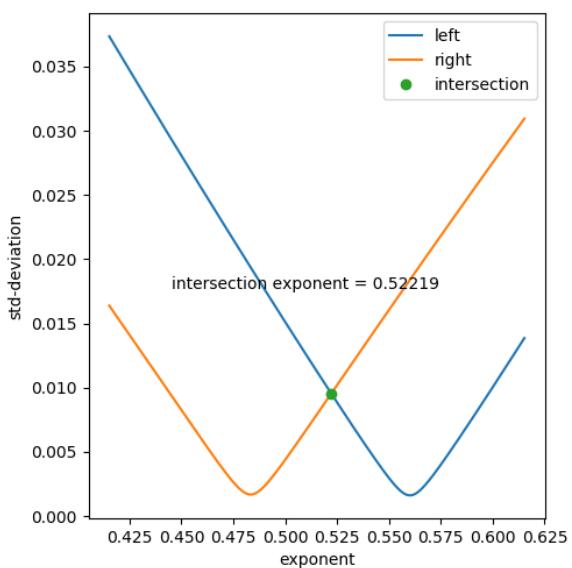


Fig. C.1 Minimizing exponent for scaling x -values

Appendix D

Measuring Entropy Efficiently

In percolation we measure the Shannon entropy [121] to measure entropy of a system. But measuring Shannon entropy is very costly. Since we have to measure entropy for each value of p (total L^2 iteration in site percolation) and there can be at most $2L^2$ cluster in site percolation (initial state). Therefore it would cost as $\mathcal{O}(L^2m)$ where $1 \geq m \geq 2$. Which is not good for taking 1000s of ensemble.

To improve the entropy measuring system we can do the following: we measure entropy initially in the traditional way (taking sum over all the clusters) and call it H_{old} . We then select a site and without occupying it measure the entropy of the cluster that is related to the site first and call it H_s . Then we occupy the site and measure the entropy of the cluster that emerges after occupying the site and call it H_a . Therefore at this point the entropy of the system is

$$H = H_{old} - H_s + H_a \quad (\text{D.1})$$

Then we set $H_{old} = H$ and repeat the process. This way we don't need to measure entropy for each cluster at each iteration, we only need to measure the change in entropy. Recall that $mu_i = \frac{S_i}{\sum_i S_i}$ where S_i is the size of the i -th cluster and $\sum_i S_i = M = 2L^2$ in site percolation.

At this point an worked out example is helpful. Say we have a lattice of length $L = 8$ then there are $N = 64$ sites and $M = 128$ bonds D.1. And initially there are M clusters of size

1 (only one bond per cluster). Then the initial entropy H_{init} is

$$\begin{aligned}
 H_{init} &= -\sum_i \mu_i \log_2 \mu_i \\
 &= -128 \times \frac{1}{128} \log_2 \frac{1}{128} \\
 &= -\log_2 \frac{1}{128} \\
 H_{init} &= \log_2 128 = 7.0
 \end{aligned} \tag{D.2}$$

Since $\mu_i = 1/128$ When we occupy one site it will connect with four bonds to create a cluster of size 4.

$$\begin{aligned}
 H_s &= -\sum_{i=1}^4 \frac{1}{128} \log_2 \frac{1}{128} \\
 &= \frac{4}{128} \log_2 (128) = 0.21875
 \end{aligned} \tag{D.3}$$

$$\begin{aligned}
 H_a &= -\frac{4}{128} \log_2 \frac{4}{128} \\
 &= \frac{4}{128} \log_2 \frac{128}{4} = 0.15625
 \end{aligned} \tag{D.4}$$

Therefore

$$\begin{aligned}
 H_{new} &= H_{init} - H_s + H_a \\
 &= \log_2 (128) - \frac{4}{128} \log_2 (128) + \frac{4}{128} \log_2 \frac{128}{4} \\
 &= 6.9375
 \end{aligned} \tag{D.5}$$

In the same system after some time there will be less small cluster and more large. Say we are in a state of the system consists of 2 large cluster. We mark them as green and red cluster. Then entropy for green and led cluster is

$$H_{green} = -\frac{13}{128} \log \frac{13}{128} \tag{D.6}$$

$$H_{red} = -\frac{7}{128} \log \frac{7}{128} \tag{D.7}$$

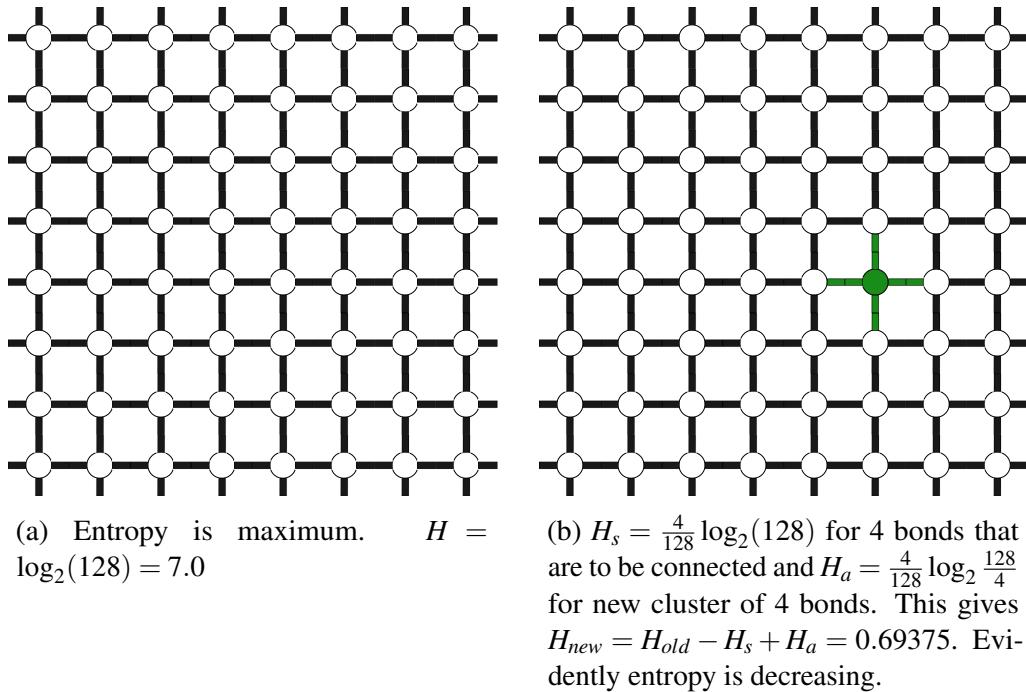


Fig. D.1 Entropy of a system in initial state and one step after it.

Since $S_{green} = 13$ and $S_{red} = 7$. And all other clusters are of size 1. Therefore the entropy of the clusters of size 1 is

$$H_{one} = - \sum_{i=1}^{128} 128 - 7 - 13 \frac{1}{128} \log_2 \frac{1}{128} = \frac{108}{128} \log_2 128 \quad (\text{D.8})$$

Thus the total entropy is $H = H_{one} + H_{green} + H_{red}$ (see figure D.2a).

Now say we select the site connecting green and red cluster to occupy. Then

$$H_s = H_{green} + H_{red} \quad (\text{D.9})$$

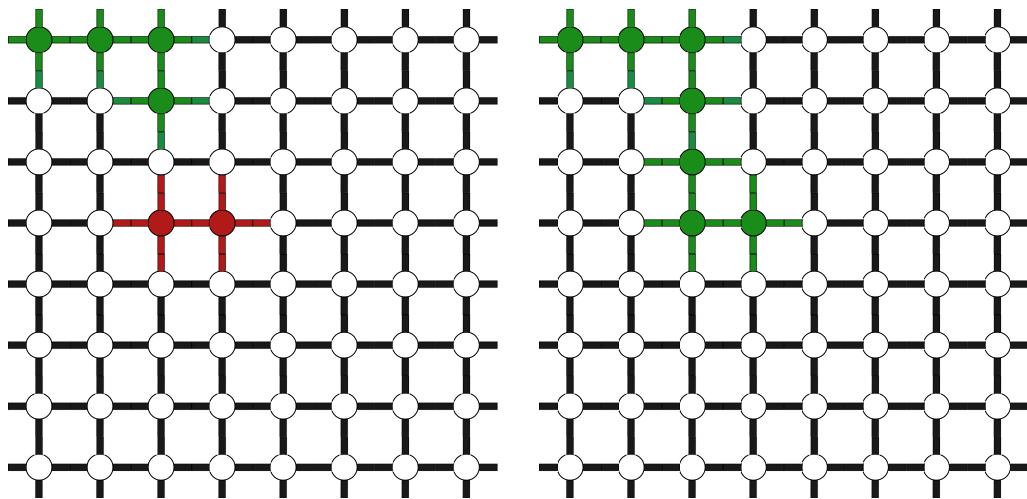
and

$$H_a = - \frac{22}{128} \log_2 \frac{22}{128} \quad (\text{D.10})$$

since size of the new cluster after occupying the selected site is 22.

Then the entropy of the system is

$$H = H_{one} \quad (\text{D.11})$$



$$(a) H_{old} = H_{one} + H_{green} + H_{red}$$

$$(b) H_{new} = H_{old} - H_s + H_a \text{ where } H_s = H_{green} + H_{red} \text{ is to be found from figure D.2a}$$

Fig. D.2 Entropy of a system in a middle state and one step after.

D.2b.