Percolation by a class of ballistic deposition and their universality classes



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This dissertation is submitted for the degree of *Masters of Physics*

December 2018



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 Acknowledgements. This dissertation contains fewer than 65,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 150 figures.

Muhammad Shahnoor Rahman December 2018

Acknowledgements

And I would like to acknowledge ...

Abstract

This is where you write your abstract ...

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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. Later, in 1957 it acquires the mathematical formulation due to the work of engineer Simon Broadbent and mathematician John Hammersley. Ever since then percolation theory has been studied extensively by scientists in general and physicits in particular.

- 1.1 Motivation and Objective
- 1.2 Method of Study
- 1.3 Organization of Chapters

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 inadequate 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, ince 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 $[\rho] = FL^{-4}T^{-2}$? [3].

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, \ldots 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 n dimensionless variable problem if each of the n dimensional variable of original n variables can be expressed in terms of the n-k dimensionally independent variable.

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

$$a = f(a_1, a_2, \dots, a_3)$$
 (2.1)

where the quantities $a_1, a_2, ..., a_n$ 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 $a_{k+1}, ..., a_n$ have the independent dimensions and the dimensions of the arguments $a_1, a_2, ..., a_k$ can be expressed in terms of the dimensions of the governing independent parameters $a_{k+1}, ..., a_n$ in the following way

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

$$[a_2] = [a_{k+1}]^{\alpha_2} \dots [a_n]^{\gamma_2}$$
(2.2)

$$[a_k] = [a_{k+1}]^{\alpha_k} \dots [a_n]^{\gamma_k}$$
(2.3)

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

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

$$(2.4)$$

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

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

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

$$\vdots (2.7)$$

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

and a dimensionless governed parameter

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

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

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

The quantities $\Pi, \Pi_1, \ldots, \Pi_k$ 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}, \ldots, 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 $\frac{\delta F}{\delta a_{k+2}} = 0, \ldots, \frac{\delta F}{\delta a_n} = 0$. Therefore, the relation 2.10 is in fact represented by a function of k arguments and proves it is independent of a_{k+1}, \ldots, a_n , that is,

$$\Pi = \Phi(\Pi_1, \dots, \Pi_k) \tag{2.11}$$

and the function f can be written in the following special form

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

$$S = S(a, b, c) \tag{2.13}$$

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

$$[a] \sim [c]$$
 and $[b] \sim [c]$ (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

$$\Pi_1 = \sin \theta = a/c \tag{2.15}$$

$$\Pi_2 = \cos \theta = b/c \tag{2.16}$$

and the dimensionless governed paremeter

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

$$\Pi = \phi(\Pi_1, \Pi_2) \tag{2.18}$$

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

$$S = c^2 \phi(\theta) \tag{2.19}$$

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

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

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

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

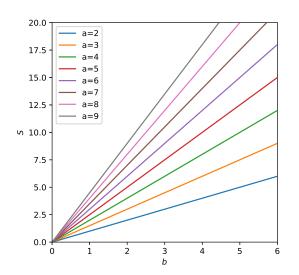
since the numerical value of the ratio of the area over the square of the hypotenuse depends on the angle θ . It implies that if we plot the ratio of the area over the square of the hypotenuse as a function θ all the data points should collapse onto a single curve regardless of the size of the hypotenuse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

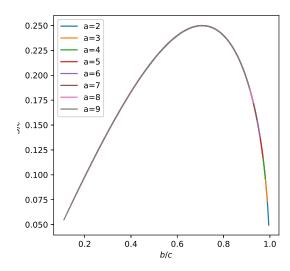
$$\phi(b/c) = \frac{1}{2}\sin\theta\tag{2.22}$$

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,





- (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

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, \ldots, 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 the same when compared. This also means that a self-similar structure is infinite in theory. Therefore 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 wasting 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

$$\alpha = f(a_1, a_2, a_3, b_1, b_2) \tag{2.23}$$

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

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

and for model we have

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

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

and

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

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.,

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

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

It also follows that the governed dimensionless parameter satisfies

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

Returning to dimensional variables, we get from the above equation

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

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

and

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



(a) A cauliflower



(b) Disection of cauliflower

Fig. 2.2 Self-Similarity in Cauliflower

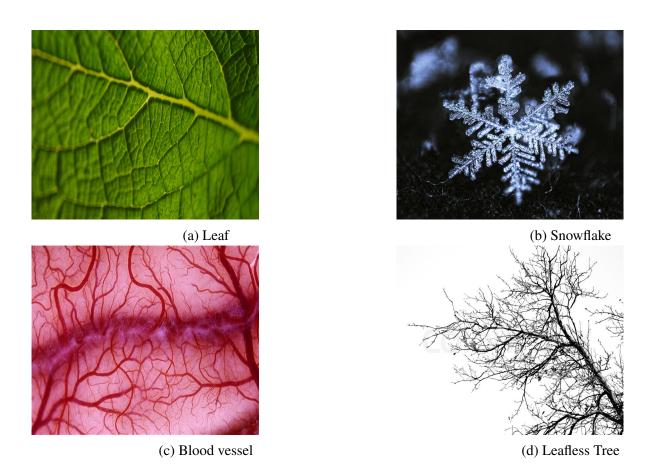


Fig. 2.3 Self-Similarity examples

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.

2.4 Scaling Hypothesis

2.4.1 Dynamic Scaling

A function f(x,t) is said to obey dynamic scaling if one of the variable t strictly denotes time and if it satisfies

$$f(x,t) \sim t^{\theta} \phi(x/t^{z}) \tag{2.34}$$

where 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

$$f(x,t) \sim x^{\omega} \phi(x/t^z) \tag{2.35}$$

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

$$x \to \lambda^z x$$
 (2.36)

$$t \to \lambda t$$
 (2.37)

$$f \to \lambda^{\theta}$$
 (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

$$x \sim t^{z} \tag{2.39}$$

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 depend 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

There exists another scaling hypothesis, known as the finite-size scaling (FSS), that 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

$$M \sim (T - T_c)^{\beta} \tag{2.40}$$

$$\chi_M \sim (T - T_c)^{-\gamma} \tag{2.41}$$

$$C_V \sim (T - T_c)^{-\alpha} \tag{2.42}$$

$$\xi \sim (T - T_c)^{-\nu} \tag{2.43}$$

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

$$f(\varepsilon, L) \sim L^{-\omega/nu} \phi(\varepsilon L^{1/\nu})$$
 (2.44)

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 $L \to \infty$ 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

$$\pi = \frac{L}{\xi} = L(T - T_c)^{\nu} \tag{2.45}$$

and the corresponding dimensionless governing parameter is

$$\Pi = \frac{f(\varepsilon, L)}{\xi \omega} = \phi(\pi) \tag{2.46}$$

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

$$f(\varepsilon, L) \sim (T - T_c)^{-\nu \omega} \phi(L(T - T_c)^{\nu})$$
 (2.47)

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

$$f(\varepsilon, L) \sim L^{\theta} \phi(\{L(T - T_c)^{\nu}\}^{-1}) \tag{2.48}$$

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

$$\pi^{1/\nu} = (L/\xi^{1/\nu}) = (T - T_c)L^{1/\nu}$$
(2.49)

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

$$f(\varepsilon, L) \sim L^{\theta} \phi((T - T_c)L^{1/\nu})$$
 (2.50)

which is the same as the traditional scaling form given by 2.44 if we find θ negative and it is related to the exponent v via $\theta = -\omega/v$.

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 $L \to \infty$. 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

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

$$f(\lambda x) = g(\lambda)f(x) \,\forall \lambda \tag{2.51}$$

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 2.51 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 2.51 can be written as

$$f(\lambda x) = \frac{f(\lambda)f(x)}{f(1)}$$
 (2.52)

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

$$xf'(\lambda x) = \frac{f'(\lambda)f(x)}{f(1)}$$
 (2.53)

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

$$xf'(x) = \frac{f'(1)f(x)}{f(1)}$$
 (2.54)

This is a first order differential equation which has a solution

$$f(x) = f(1)x^{-\alpha} (2.55)$$

where $\alpha = -f(1)/f'(1)$. There it is proven that the power law is the only solution that can satisfy 2.51. 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 $\frac{f(\lambda r)}{f(x)}$ 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.

2.5.1 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,

$$f(\lambda^a x, \lambda^b y) = \lambda f(x, y) \tag{2.56}$$

where a,b are arbitrary numbers. In contrast to the homogeneous functions defined in the previous section ?? generalized homogeneous functions can not be written as $f(\lambda x, \lambda y) = \lambda^p f(x,y)$, because 2.56 can not be generalized any further to the following form,

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x, y) \tag{2.57}$$

choosing p = 1 in the above equation yields

$$f(\lambda^{a/p}x, \lambda^{b/p}y) = \lambda f(x, y)$$
 (2.58)

Similarly an statement converse is also valid and the equation above is no more general than the form in the equation 2.56. Another equivalent form of 2.56 is as follows,

$$f(\lambda x, \lambda^b y) = \lambda^p f(x, y) \tag{2.59}$$

Similarly

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

Note that there are at least two undetermined parameters a and b for a generalized homogeneous function. Now let use see what happens if we choose $\lambda^a = 1/x$ to set in equation 2.56,

$$f(1, \frac{y}{x^{b/a}}) = x^{-\frac{p}{a}} \tag{2.61}$$

$$f(x,y) = x^{p/a} f(y/x^{b/a})$$
 (2.62)

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This combining and hence the simplification of two variables x and y into a single term has far reaching consequence in Windom scaling ?? in the theory of phase transition and critical phenomena.

Chapter 3

Phase Transition

What is this Phase transition is one of the most studied problem 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.

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.

$$\Delta E = Q + W \tag{3.1}$$

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

$$dE = dQ - PdV (3.2)$$

E 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

$$dQ = TdS?? (3.3)$$

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

$$dE = TdS - pdV (3.4)$$

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

$$dE = TdS - pdV + \mu dN \tag{3.5}$$

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

$$dE = TdS - pdV$$

$$= TdS + SdT - SdT - PdV$$

$$d(E - TS) = -SdT - PdV$$

$$dA = -SdT - PdV$$
(3.6)

where A = A(T, V) is the Helmholtz free energy. We can perform another Legendre transformation in 3.6 as follows

$$dA = -SdT - PdV - VdP + VdP$$

$$d(A + PV) = -SdT + VdP$$

$$dG = -SdT + VdP$$
(3.7)

3.1 Classification 23

where G = G(T, P) is the Gibbs free energy. Let's take a break to talk about free energy. What is free energy?

3.1 Classification

3.1.1 First Order

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

3.1.2 Second Order

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

3.2 Thermodynamic Quantities

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 [33].

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 temprature 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 ot 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.

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 [11].

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

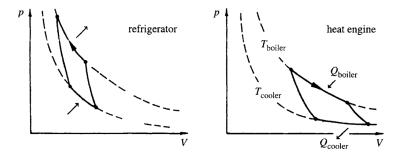


Fig. 3.1 Two competing Carnot engines, pressure (P) versus volume (V) - diagrams [10]

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 [26].

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 [23]. It is easy to calculate the efficiency of the Carnot engine of an ideal gas:

$$\eta = \frac{W}{Q_{boiler}} \\
= \frac{Q_{boiler} - Q_{cooler}}{Q_{boiler}} \\
= 1 - \frac{Q_{cooler}}{Q_{boiler}} \\
= 1 - \frac{T_{cooler}}{T_{boiler}} \tag{3.8}$$

where *T* is the Kelvin temperature. And, since by Clausius' 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

$$dU = dQ - dW (3.10)$$

$$= dQ - PdV \tag{3.11}$$

since

$$dW = PdV (3.12)$$

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 3.9

$$\frac{Q}{T}\Big|_{\text{boiler}} = \frac{Q}{T}\Big|_{\text{heater}}$$
 (3.13)

nd decided to define the entropy change to be the ratio of heat flow to temperature: [77]

$$\Delta S_{\text{thermo}} = \frac{Q}{T} \tag{3.14}$$

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

$$dS \ge \frac{dQ}{T} \tag{3.15}$$

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 3.15. We may then eliminate dQ between the first and second laws, we obtain the Gibbs equation

$$dS = \frac{1}{T} \left(dU + PdV \right) \tag{3.16}$$

In an adiabatic irreversible process, dQ = 0 and equation 3.15 one has the fundamental relation between entropy and irresponsibility. In words

In a closed system (adiabatic), the entropy cannot decrease, it remains constant or increase [14] 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 [77].

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 [77]. 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 where 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 [72]. The Boltzmann entropy formula or Boltzmann-Planck entropy formula is

$$S = k_B \log \Omega \tag{3.17}$$

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 $1.4 \times 10^{-23} \ J/K$), 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 3.17, the entropy S increases when Ω does. The more microstates are, the more disorder and more entropy are. 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 [11].

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 [9].

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 [78]. This process of getting Shannon entropy from Boltzmann entropy and how does it help us is described in section 4.5.3.

3.2.2 latent heat

The latent heat associated with the phase transition is, where and are the entropies just above and below the phase transition. Since the entropy is continuous at the phase transition, the latent heat is zero. The latent heat is always zero for a second order phase transition.

3.2.3 Specific Heat

The specific heat is the amount of heat per unit mass required to raise the temperature by one degree Celsius. The relationship between heat and temperature change is usually expressed in the form shown below where *C* is the specific heat.

$$C = \frac{Q}{dT} \tag{3.18}$$

and we know

$$Q = TdS (3.19)$$

where S is the entropy. we immediately get

$$C = T \frac{dS}{dT} \tag{3.20}$$

3.2.4 Order Parameter

3.2.5 Susceptibility

The first law of thermodynamics for a non magnetic system is ??

$$dE = TdS - PdV (3.21)$$

for a magnetic system $P \to h$ and $V \to -m$, 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

$$dE = TdS + hdm (3.22)$$

$$= TdS + SdT - SdT + hdm (3.23)$$

$$d(E - TS) = -SdT + hdm (3.24)$$

$$dA = -SdT + hdm (3.25)$$

$$dA = -SdT + hdm + mdh - mdh (3.26)$$

$$d(A - mh) = -SdT - mdh (3.27)$$

$$dG = -SdT - mdh (3.28)$$

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 3.28 3.25 we can find the expression for entropy and magnetization in terms of free energy.

$$S = -\left(\frac{\partial G}{\partial T}\right)_h = -\left(\frac{\partial A}{\partial T}\right)_m \tag{3.29}$$

$$m = -\left(\frac{\partial G}{\partial h}\right)_T \tag{3.30}$$

$$h = \left(\frac{\partial A}{\partial m}\right)_T \tag{3.31}$$

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

$$\chi = \left(\frac{\partial m}{\partial h}\right)_h = -\left(\frac{\partial^2 G}{\partial h^2}\right)_T \tag{3.32}$$

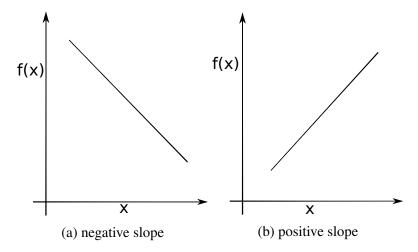


Fig. 3.2 shape of f(x) from f'(x)

again we can write χ as

$$\chi = \frac{1}{\frac{\partial h}{\partial m}}
= \frac{1}{\frac{\partial^2 A}{\partial m^2}}$$
(3.33)

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.

3.3.2 Free Energy

Now since we obtain from 3.7 that the entropy is the first derivative of the free energy 3.34 and from 3.39 specific heat is the second derivative of the free energy 3.35. Now 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

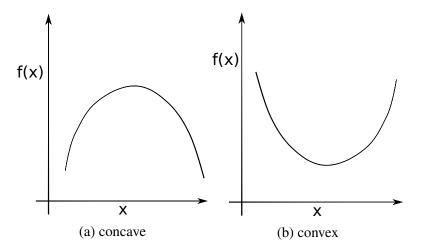


Fig. 3.3 shape of f(x) from f''(x)

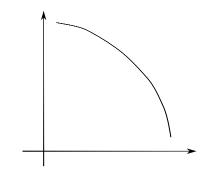


Fig. 3.4 Shape of the free energy

that the shape of the free energy should be a decreasing concave curve 3.4 in other words concave shaped with negative slope.

$$S = -\frac{\partial G}{\partial T} \tag{3.34}$$

$$C = -\frac{\partial^2 G}{\partial T^2} \tag{3.35}$$

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.

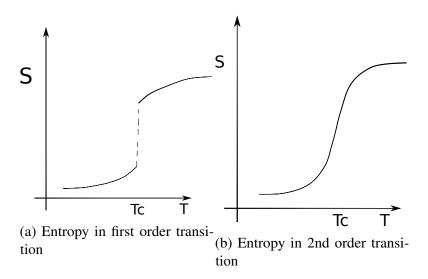


Fig. 3.5 Shape of entropy

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 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 3.37. Using this and the shape of entropy we can get the shape of the specific heat immediately as follows

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 3.32 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 3.30 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 3.33 we can say $\frac{\partial^2 A}{\partial m^2}$ is positive giving convex shape of the Helmholtz free energy.

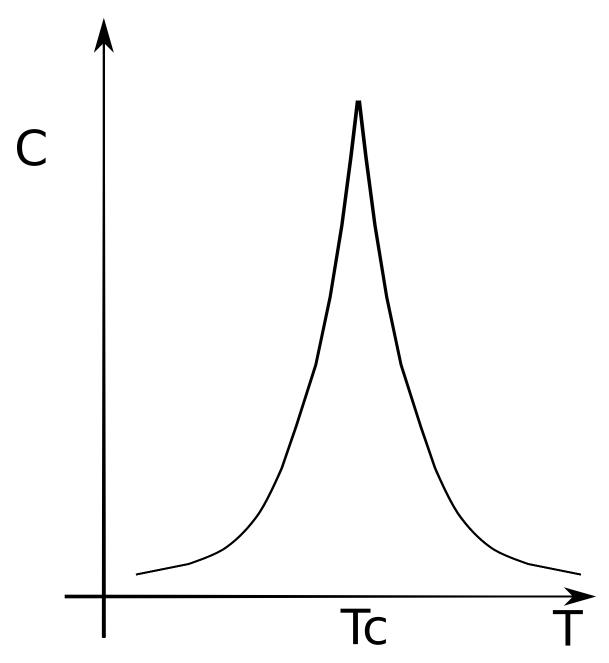


Fig. 3.6 Shape of Specific Heat

And 3.31 tells us that since h can ve positive or negative, the Helmholtz free energy can have increasing or decreasing slope respectively.

3.4 Response Functions

The Specific heat and Susceptibility are called the response function in thermodynamics and the definitions are as follows. The specific heat C_p or C_v is the derivative of the enthalpy with respect to the temperature at constant pressure or volume respectively.

$$C_{x} = \left(\frac{dQ}{dT}\right)_{x} \tag{3.36}$$

here x can be P for pressure or V for volume. And from $\ref{eq:property}$ we can write

$$C_{x} = T\left(\frac{dS}{dT}\right) \tag{3.37}$$

To give the following

$$C_{v} = -T \left(\frac{\partial^{2} A}{\partial T^{2}} \right)_{v} \tag{3.38}$$

$$C_p = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_p \tag{3.39}$$

Nearest neighbor interation and 2nd nearest neighbor interaction. Old models of phase transition: Ising model 1D and 2D. Bragg Willium model.

3.5 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

$$\varepsilon = \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1 \tag{3.40}$$

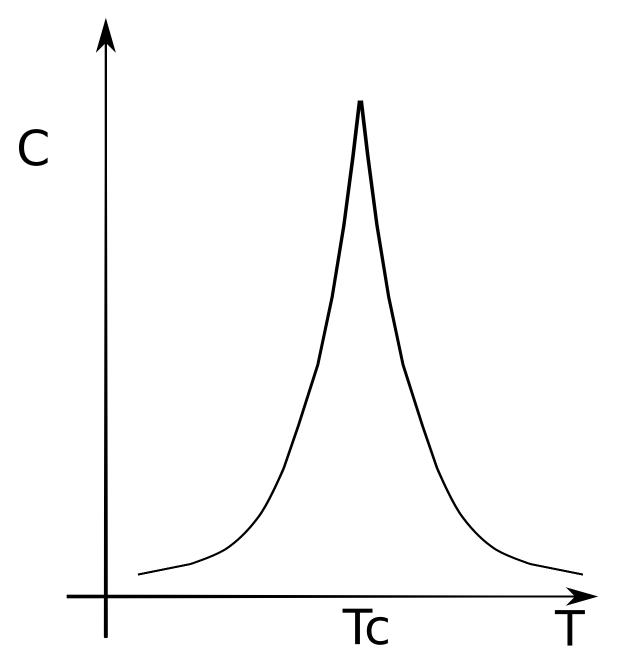


Fig. 3.7 figure required

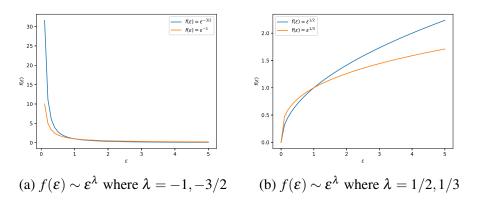


Fig. 3.8 Function showing power law

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

$$f(\varepsilon) \sim \varepsilon^{\lambda}$$
 (3.41)

The following figures shows some function that exhibit power law To see this more closely, we can expand any function $f(\varepsilon)$ as a power series of ε

$$f(\varepsilon) = A\varepsilon^{\lambda} (1 + B\varepsilon^{a} + C\varepsilon^{b} + \dots)$$
 (3.42)

Near T_c only the first term is dominating ??.

We had the Gibbs free energy (for a magnetic system)

$$G = G(T, h) \equiv G(\varepsilon, h) \tag{3.43}$$

since ε is a better parameter. Assume that G is a generalized Homogeneous function. Therefore from $\ref{eq:condition}$ we can write

$$G(\lambda^{a_{\varepsilon}}\varepsilon, \lambda^{a_{h}}h) = \lambda G(\varepsilon, h) \tag{3.44}$$

differentiating equation 3.44 with respect to h

$$\frac{\partial G(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h)}{\partial h} = \lambda \frac{\partial G(\varepsilon, h)}{\partial h}$$

$$\frac{\partial G(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h)}{\partial \lambda^{a_{h}} h} \lambda^{a_{h}} = \lambda \frac{\partial G(\varepsilon, h)}{\partial h}$$

$$\lambda^{a_{h}} G'(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h) = \lambda G'(\varepsilon, h)$$

$$-\lambda^{a_{h}} m(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h) = -\lambda m(\varepsilon, h)$$

$$m(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h) = \lambda^{1-a_{h}} m(\varepsilon, h)$$
(3.45)
$$(3.46)$$

Here m is the magnetization or order parameter.

Figure of order general parameter

Setting h = 0 in equation 3.46

$$m(\lambda^{a_{\varepsilon}} \varepsilon) = \lambda^{1-a_{h}} m(\varepsilon)$$

$$m(1) = \lambda^{1-a_{h}} m(\varepsilon)$$

$$m(1) = \varepsilon^{-\frac{1-a_{h}}{a_{\varepsilon}}} m(\varepsilon)$$

$$m(\varepsilon) = \varepsilon^{\beta} m(1)$$
(3.47)

where

$$\beta = \frac{1 - a_h}{a_{\varepsilon}} \tag{3.48}$$

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

Setting $\varepsilon = 0$ in equation 3.46

$$m(\lambda^{a_h}h) = \lambda^{1-a_h}m(h)$$

$$m(1) = h^{-\frac{1-a_h}{a_h}}m(h)$$

$$m(h) = m(1)h^{\delta}$$
(3.49)

where

$$\delta = \frac{a_h}{1 - a_h} \tag{3.50}$$

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 3.44 twice with respect to ε we get the Specific Heat

$$\lambda^{2a_{\varepsilon}}G''(\lambda^{a_{\varepsilon}}\varepsilon,\lambda^{a_{h}}h) = \lambda G''(\varepsilon,h)$$

$$\lambda^{2a_{\varepsilon}}\frac{\partial G(\lambda^{a_{\varepsilon}}\varepsilon,\lambda^{a_{h}}h)}{\left(\frac{1}{T_{c}}\right)^{2}\partial T^{2}} = \lambda G''(\varepsilon,h)$$

$$\lambda^{2a_{\varepsilon}}C(\lambda^{a_{\varepsilon}}\varepsilon,\lambda^{a_{h}}h) = \lambda C(\varepsilon,h)$$
(3.51)

We have used $\varepsilon = \frac{T}{T_c} - 1$ and $d\varepsilon = \frac{1}{T_c} dT$. Now setting h = 0 we get from 3.51

$$\lambda^{2a_{\varepsilon}}C(\lambda^{a_{\varepsilon}}\varepsilon) = \lambda C(\varepsilon)$$

$$C(1) = \lambda^{1-2a_{\varepsilon}}C(\varepsilon)$$

$$= \varepsilon^{-\frac{1-2a_{\varepsilon}}{a_{\varepsilon}}}C(\varepsilon)$$

$$C(\varepsilon) = \varepsilon^{-\alpha}C(1)$$
(3.52)

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

$$\alpha = \frac{2a_{\varepsilon} - 1}{a_{\varepsilon}} \tag{3.53}$$

Again by differentiating 3.44 twice with respect to h we get the susceptibility. Then we set h = 0 to get only ε dependency.

$$\lambda \frac{\partial^{2} G(\varepsilon, h)}{\partial h^{2}} = \lambda^{2a_{h}} \frac{\partial^{2} G(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h)}{\partial h^{2}}$$

$$\lambda \chi(\varepsilon, h) = \lambda^{2a_{h}} \chi(\lambda^{a_{\varepsilon}} \varepsilon, \lambda^{a_{h}} h)$$

$$\chi(\varepsilon) = \lambda^{2a_{h}-1} \chi(\lambda^{a_{\varepsilon}} \varepsilon)$$

$$\chi(\varepsilon) = \varepsilon^{-\gamma} \chi(1)$$
(3.54)

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

$$\gamma = \frac{2a_h - 1}{a_F} \tag{3.55}$$

3.5.1 List of Thermodynamic Quantities that Follows Power Law

Critical Exponents at a glance is it better title.

The exponent that scales Specific heat is called α

$$C \sim \varepsilon^{-\alpha}$$
 (3.56)

The exponent that scales order-parameter is called β

$$m \sim \varepsilon^{\beta}$$
 (3.57)

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

$$m \sim h^{\delta}$$
 (3.58)

The exponent that scales susceptibility is called γ

$$\chi \sim \varepsilon^{-\gamma}$$
 (3.59)

Note that these quantities only follows power law near T_c .

3.5.2 Rushbrooke Inequality

$$\alpha + 2\beta + \gamma \ge 2 \tag{3.60}$$

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

$$\alpha + 2\beta + \gamma = \frac{2a_{\varepsilon} - 1}{a_{\varepsilon}} + \frac{2(1 - a_h)}{a_{\varepsilon}} + \frac{2a_h - 1}{a_{\varepsilon}}$$
$$= \frac{2a\varepsilon}{a\varepsilon}$$
$$= 2$$

Thus the Rushbrooke inequality is satisfied.

3.5.3 Griffiths Inequality

$$\alpha + \beta(1+\delta) = 2 \tag{3.61}$$

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

$$\alpha + \beta(1+\delta) = \frac{2a_{\varepsilon} - 1}{a_{\varepsilon}} + \frac{1 - a_h}{a_{\varepsilon}} \left(1 + \frac{a_h}{1 - a_h} \right)$$

$$= \frac{2a_{\varepsilon} - 1}{a_{\varepsilon}} + \frac{1}{a_{\varepsilon}}$$

$$= \frac{2a_{\varepsilon}}{a_{\varepsilon}}$$

$$= 2$$

(3.62)

So the Griffiths Inequality is also satisfied.

3.6 Models

- 3.6.1 Ising model in 1D lattice
- 3.6.2 Ising model in 2D lattice

Chapter 4

Percolation Theory

Percolation theory potentially has been of great interest as it can describe many phenomena [70]. 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. 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 disperate systems 4.9.

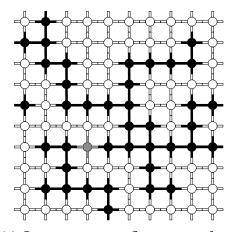
To study percolation theoretically, the first thing that one need is to choose a skeleton or playground, namely an empty lattice (or a graph/network), consisting of sites (or nodes) and bonds (or links). The definition of the percolation model is then so simple that it merely needs a sentence to define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

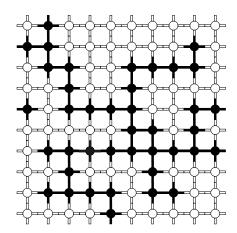
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occupied sites form a cluster, or to their distribution function. As the occupation probability p is tuned starting from p=0, one finds that at certain value of $p=p_c$ the observable quantities undergoes a sudden and sharp change which is always regarded 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 artichect 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 $r \le p$ 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 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





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- (a) One step away to flow current from top to bottom only if the gray 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 $p < p_c$.

finite and infinite range connectivity. This is actually non-trivial when the space is randomly disordered and the connected regions acquire fractal properties [82, 58].

4.2 Historical Overview

In 1941, the idea of percolation was first conceived by Flory [37] 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 [20], 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 [35, 36]. 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 [49]. This work paved the way to many exact results in percolation, and also allowed the usage of powerful re-normalization group ideas [22]. Finding percolation threshold both exactly and by simulation has been an enduring subject of research in this field [73], as well as the development of algorithms such as those by Hoshen and Kopelman [46], by Leath [52], and by Newman and Ziff [62] (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 [50], Wierman [79], Bollobas and Riordan [18] etc.) Another infusion of interest in percolation came from the surgin field of network theory which goes back to the study of random and complete graphs by Erdos-Renyi(1959). In ER

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model, an observation of made of formation of a giant component, this giant component is exactly analogous to the formation pattern in percolation [1, 34]. 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 [60]. In the field of random networks, the model of explosive percolation was first introduced by Achlioptas, D'Souza and Spencer [7], 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 $p \ge p_c$ 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 [68]. 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 [7]. 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 [76]. Determining K-cores computationally is fast and they are insightful in many situations [32, 30]. 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 >= 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 [67].

Bootstrap Percolation

Bootstrap percolation is an infection-like process in which nodes becomes infected if sufficiently many of their neighbors are infected [8]. In bootstrap percolation, sites on an empty lattice are first randomly occupied and then all occupied sits 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 $m \ge 3$, 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 [15], it is concluded that the effects like bootstrap percolation may occur in some real magnets [24].

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 [54]. 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" [65]. Various percolation processes have also been studied in several different types of multi-layer networks (e.g. multiplex networks and interdependent networks) [16, 51]. 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 [43, 66, 17], 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* [42, 57, 81]; 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 [53].

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.

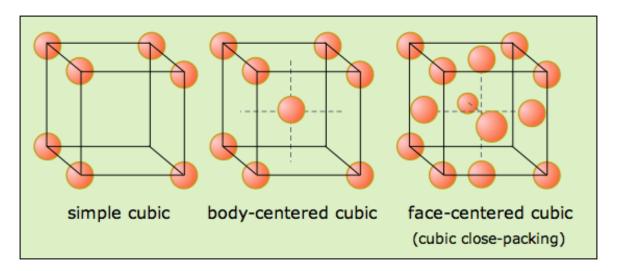


Fig. 4.2 Different types of cubic lattice [2]

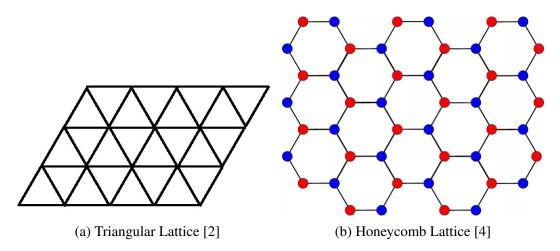


Fig. 4.3 Different types of cubic lattice

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 [55]. They calculated Fisher exponent, τ , the finite-size correction exponent, Ω and the scaling function exponent, Ω confirmed to be universal. They also did percolation on the HCP (hexagonal closed packed) lattice [56]. Before that in 1981 JC Wireman studied bond percolation on honeycomb and triangular lattices [80].

Furthermore, an exact solution on Bethe lattice for high density percolation was done by G. R. Reich and P. L. Leath in 1978 [69] and J. Chalupa et al. did bootstrap percolation on Bethe lattice in the following year [24].

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 []. 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 [6] 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 [21]. Clique percolation is also studied on random networks [31]. A critical phenomenon analysis on random networks for core percolation is done by Bauer [13]. In early 80's, before the birth of scale free networks, C McDiarmid did two significant works which you can find in the references [].

Reuvan Cohen et al. studied scale free networks close to the percolation threshold [27]. N. Schwartz et al. worked on percolation problem in directed scale free networks [74]. Filippo Radicchi and Santo Fortunato studied scale-free networks constructed via a cooperative Achlioptas Growth Process [7]. 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 4.7 we discuss who we determine p in



Fig. 4.4 Scale Free Network [5]

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 [61, 62].

4.4.2 Cluster

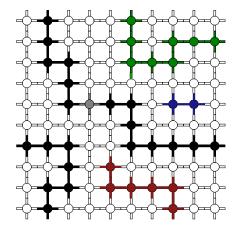
Cluster is a collection of sites and bonds. In bond percolation we occupy bond and measure cluster size in terms of the number of sites in it. And following this idea we measure the cluster size in terms of the number of bonds in it. Which is the new definition of site percolation [68]. Measuring cluster 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.

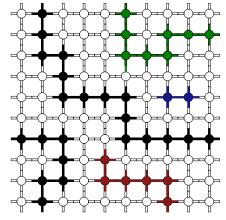
4.4.3 Spanning cluster

4.5 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 [68] With no gap or unoccupied object between them. In a network cluster

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

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.

4.5.1 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 $p \ge p_c$ 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 threshold has been determined for different types of lattices. The table 4.1 shows some of them.

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

$$p_{c_a vg} = \lim_{M \to \infty} \frac{1}{M} \sum_{i} p_{c_i}$$
 (4.1)

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

But performing infinite number of experiment is not possible. So we use another approach which is described in section 4.5.2 and 5.4.1

4.5.2 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 $p_{c_i} \le p \le 1$. 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 [68]. Figure 5.1 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 $L \to \infty$ 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 $(p-p_c)L^{1/\nu}$ we would get a perfect data collapse for a specific 1/nu that is our exponent. This process is discussed further in section 5.4.1 and 5.4.2.

4.5.3 Entropy, H(p,L)

Entropy in one of the key feature 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

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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 [78]. The seminal work of Shannon based on papers by Nyquist [63, 64] and Hartley [44]. He rationalized these early efforts into a coherent mathematical theory of communication.

The Defition of Shannon entropy is

$$H = -\sum_{i} \mu_{i} \log \mu_{i} \tag{4.2}$$

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

As we have seen in section 3.2.1 that the entropy measures disorderness 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'_1 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

$$\Omega = \frac{M!}{\left(M_{\mu_1}\right)! \left(M_{\mu_2}\right)! \dots \left(M_{\mu_m}\right)!} \tag{4.3}$$



(a) Entropy of this system is in minimum



(b) Entropy of this system is in between maximum and minimum



(c) All distinct cluster. A system of maximum entropy

Fig. 4.6 A system of 12 cluster

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

$$\log \Omega = \log M! - \log \left(\prod_{i} M_{\mu_{i}} \right)$$

$$= M \log M - M - \sum_{i} \log \left(M_{\mu_{i}}! \right)$$

$$= M \log M - M - \sum_{i} \left[M_{\mu_{i}} \log M_{\mu_{i}} - M_{\mu_{i}} \right]$$

$$= M \log M - \sum_{i} M_{\mu_{i}} \log M_{\mu_{i}}$$

$$= M \log M - M \sum_{i} \frac{M_{\mu_{i}}}{M} \left[\log \left(\frac{M_{\mu_{i}}}{M} \right) + \log M \right]$$

$$= M \log M - M \sum_{i} \mu_{i} \log \mu_{i} + M \sum_{i} \frac{M_{\mu_{i}}}{M} \log M$$

$$(4.4)$$

Finally we have,

$$\log \Omega = -M \sum_{i=1}^{m} \mu_i \log \mu_i = MH(\mu)$$
(4.5)

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 [68]. Now recall the definition of Boltzmann entropy in equation 3.17. If we consider $K_B = 1$ then we get Shannon entropy to represent Boltzmann entropy.

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

$$H = -(0.5\log_2(0.5) + 0.5\log_2(0.5))$$
$$= -(0.5 \times (-1) + 0.5 \times (-1))$$
$$= 1$$

so in this system entropy is 1.

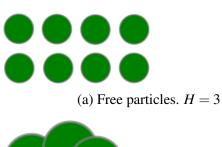
Now take a new system where there is 4 identical object. Since all objects are identical, each have probability $\mu_i = 1/4$ and $\log_2(1/4) = -2$. Then the total entropy of that system is 2. So this is clear that the entropy increses with the increase of the system size. Here system size is determined 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,

$$\begin{split} H &= -\sum_{i} \mu_{i} \log_{2} \mu_{i} \\ &= -(4/8 \log_{2}(4/8) + 2/8 \log_{2}(2/8) + 1/8 \log_{2}(1/8) + 1/8 \log_{2}(1/8) \\ &= -(-1/2 - 1/2 - 3/8 - 3/8) \\ &= 7/4 \end{split}$$

which is less then 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.

4.5.4 Specific Heat, C(p,L)

According to the definition of specific heat in thermodynamics 3.20 we can find specific heat if we know the temperature and entropy. In percolation theory we measure the Shannon





(b) Some Free and Some Bound Particles. 0 < H < 3



(c) Bount particles. H = 0

Fig. 4.7 entropy of a system of 8 particles

entropy, H(p,L). And we use (1-p) as the analogue of temperature which gives

$$C = (1 - p)\frac{dH}{d(1 - p)} \tag{4.6}$$

$$= -(1-p)\frac{dH}{dp} \tag{4.7}$$

using this definition we can easily find the specific heat of the percolating system. And from specific heat we obtain the critical exponent α .

4.5.5 Order Parameter, P(p,L)

From above discussion we can say that if $p \ge p_c$ 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).

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We define the percolation strength as

$$P = \frac{\text{number of sites in the spanning cluster}}{\text{total number of sites in the lattice}}$$
(4.8)

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

$$P = \frac{\text{number of nodes in the largest cluster}}{\text{total number of nodes in the network}}$$
(4.9)

Both definition, though looks a bit different when plotted, gives the same critical exponent β . How to find this exponent is shown in section 5.4.4.

Mathematically

$$P(p,L) = \frac{K}{\sum_{i} k_{i}} \tag{4.10}$$

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

$$\sum_{i} k_i = L^2 \tag{4.11}$$

and without periodic boundary condition

$$\sum_{i} k_{i} = L(L-1) \tag{4.12}$$

- **4.5.6** Susceptibility, $\chi(p,L)$
- 4.5.7 Mean Cluster Size, S
- 4.5.8 Cluster Size Distribution Function, n_s

$$n_s(p_c) \sim s^{-\tau} \tag{4.13}$$

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

- **4.5.9** Correlation Function, g(r)
- 4.5.10 Correlation length, ξ
- **4.5.11** Fractal Dimension, d_f

4.6 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 a 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.

4.6.1 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.

$$\lim_{L \to \infty} omega(p, L) = \begin{cases} 0, \forall p < 1 \\ 1 \text{ only if p = 1} \end{cases}$$
 (4.14)

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For p=1 all sites of the lattice are occupied and a percolating cluster spans from $-\infty$ to ∞ so that each and every and every sites of the lattice belong to the percolating cluster. For p<1 we will have on the average $(1-p)^L$ empty sites. So if $L\to\infty$, we have $(1-p)^L\to const$. 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

$$p_c = 1 \tag{4.15}$$

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 are 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

$$n_s = p^s (1 - p)^s (4.16)$$

 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 4.16 gives

$$n_s = (1 - p)^2 \exp(s \ln p) = (1 - p)^2 \exp(-s/\xi)$$
(4.17)

where ξ is the correlation length and defined as

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln(p_c - (p_c - p))} \sim (p - p_c)^{-1} = (p - p_c)^{\nu}$$
 (4.18)

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

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to the probably p that it is occupied.

$$\sum_{s=1}^{\infty} sn_s = \frac{number of total occupied sites}{number of total lattice sites} = p$$
(4.19)

A quick check of the validity of equation 4.19 can be performed using equation 4.16.

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

$$= (1-p)^2 \sum_s s p^s$$

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

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

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

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

$$= p$$
(4.20)

Here we have used the series sum 4.21.

$$\sum_{s} p^{s} = p + p^{2} + p^{3} + \dots$$

$$= p(1 + p + p^{2} + \dots)$$

$$= p(1 - p)^{-1}$$
(4.21)

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

$$w_s = \frac{n_s s}{\sum_s n_s s} \tag{4.22}$$

 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

$$S = \sum_{s} w_s s \tag{4.23}$$

This equation is very much similar to

$$\bar{x} = \int x p(x) dx \tag{4.24}$$

using equation 4.22 we get

$$S = \frac{\sum_{s} n_{s} s^{2}}{\sum_{s} n_{s} s}$$

$$= \sum_{s=1}^{\infty} \frac{s^{2} n_{s}}{p}$$

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

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

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

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

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

$$= p(1-p)^{2} 2(1-p)^{-3}$$

$$= \frac{2p}{1-p}$$

$$= \frac{1+p}{1-p}$$

$$= (4.25)$$

we can write

$$S(p) = \frac{1-p}{1+p} = \frac{p_c + p}{p_c - p} \tag{4.26}$$

using the fact that $p_c=1$ in 1D lattice. This equation reveals that the mean cluster size diverges for $p\to p_c$ 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 [45]

$$S(p) \sim (p_c - p)^{-1}$$
 (4.27)

We encounter the similar behaviour in the higher dimensions also.

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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

$$g(r) = p^r \tag{4.28}$$

It can also be expressed in terms of correlation length ξ

$$g(r) = \exp(\ln(p^r)) = \exp(-r/\xi)$$
 (4.29)

where ξ is the correlation length 4.18.

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

$$S = 1 + \sum_{r=1}^{\infty} g(r) \tag{4.30}$$

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.

4.6.2 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

$$A \propto V^{1-1/d} \tag{4.31}$$

now as $d \to \infty$ we have

$$A \propto V \tag{4.32}$$

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 number of sites in the Bethe lattice is

$$1 + 3 \times (1 + 2 + \dots + 2^{r-1}) = 3 \cdot 2^r - 2 \tag{4.33}$$

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

$$1 + 2 + 2^2 + 2^3 + \ldots + 2^r = 2^{r+1} - 1 \tag{4.34}$$

And if we measure the surface to volume ratio we get

$$\frac{A}{V} = \frac{number of sites in the surface}{total number of sites} = \frac{3 \times 2^{r-1}}{3 \times 2^r - 2}$$
(4.35)

as $r \to \infty$ we get

$$\frac{A}{V} \sim \frac{3 \times 2^{r-1}}{3 \times 2^r} = \frac{1}{2} = constant \tag{4.36}$$

Therefore Bethe lattice is indeed an infinite dimensional lattice.

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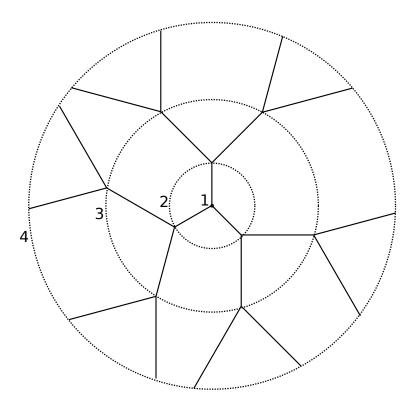


Fig. 4.9 Bethe Lattice for z = 3

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 $r \to \infty$ 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

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

$$p_c = \frac{1}{z-1}$$
(4.37)

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

$$P(p) = p(1 - Q^3) (4.38)$$

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,

$$Q = (1 - p) + pQ^2 (4.39)$$

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

$$Q = 1, \frac{1 - p}{p} \tag{4.40}$$

For z neighbors, in general we have

$$Q = 1, 1 - \frac{2p(z-1) - 2}{p(z-1)(z-2)}$$
(4.41)

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 $p = p_c = 1/2$

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p \left(1 - \left(\frac{1-p}{p} \right)^3 \right) & \text{for } p \ge p_c \end{cases}$$
 (4.42)

Let,

$$f(p) = \left(\frac{(1-p)}{p}\right)^3\tag{4.43}$$

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Then

$$f'(p) = -3p^{-4}(1-p)^{3} - 3p^{-3}(1-p)^{2}$$

$$= -\frac{3}{p} \left(\frac{(1-p)}{p}\right)^{3} - \frac{3}{p} \left(\frac{(1-p)}{p}\right)^{2}$$
(4.44)

$$P(p) = P(p_c) + (p - p_c)P'(p_c) + \dots (4.45)$$

$$= 0 + (p - p_c) (1 - f(p_c) - pf'(p_c)) + \dots$$
 (4.46)

$$=6(p-p_c)+\dots \tag{4.47}$$

(4.48)

Therefore we get

$$P(p) \propto (p - p_c) \text{ for } p \to p_c^+$$
 (4.49)

the critical exponent β is defined by

$$P(p) \propto (p - p_c)^{\beta} \tag{4.50}$$

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,

$$T = (1 - p) \times 0 + p(1 + 2T) \tag{4.51}$$

Solving this we get

$$T = \frac{p}{1 - 2p} \tag{4.52}$$

for $p < p_c$.

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

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Therefore the mean cluster size S(p) is

$$S(p) = 1 + 3T$$

$$= \frac{1+p}{1-2p}$$

$$= \frac{1+p}{2(p_c - p)}$$

$$= \frac{1+p}{2}(p_c - p)^{-1}$$
(4.54)

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 $p \to p_c$.

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

$$g(r) = z(z-1)^{r-1}p^r (4.55)$$

$$= \frac{z}{z-1} (p(z-1))^r \tag{4.56}$$

$$= \frac{z}{z-1} \exp[\log[p(z-1)]]$$
 (4.57)

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 $r \to \infty$. 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 4.18

$$\xi = \frac{-1}{\log[p(1-z)]}$$

$$= \frac{-1}{\log(p/p_c)}$$

$$= (p-p_c)^{-1}$$
(4.58)

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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.

4.7 Algorithm

In the classical Hosen-Kopelman algorithm for percolation model [46], one first choose an occupation probability p and then generate a number r for each site of the lattice. The site is occupied if $r \le p$ 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 very in each realization. However, the expected or ensemble average over m experiments will give m = p in the limit m. Thus the number of occupied bonds or sites is also a measure of p. Using this idea Ziff and Newman [62] proposed an algorithm which generate states for each value of m from zero up to some maximum value $m = L^2$ for site percolation on m is m and m in the limit m in the limit m is a some effort by noticing the fact that a new state with m is occupied sites or bonds can be created by adding one extra randomly chosen site or bond to the state containing m 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 Relation of Phase Transition with Percolation

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 [12]. 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 [59].

Before that in 2000, Moore et al. studied some simple models of disease transmission on small-world networks [60]. 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 [47].

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 [71].

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 [41]. 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 $\beta \simeq 0.65$ [19].

It is easiest to understand percolation theory by explaining its use in epidemiology [60]. 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.,

4.9 Application 69

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 [41] 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 [48] 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 [25]. 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, **70** Percolation Theory



Fig. 4.10 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.

and the process is equivalent to site percolation [29]. 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 [28, 75]. 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 [40, 38, 39], 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 4.9 Application 71

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 [75, 28].

Definitions of some quantities used in percolation. Basic Algorithm

4.9.5 Square Lattice

A square lattice is an ideal playground for percolation. If it has length L then number of sites in the lattice is L^2 and number of bonds in the lattice is $2L^2$. 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. If the sites are densely spaced the experiment will be accurate, meaning, the larger the size of the lattice the accurate the results will be. It implies that a lattice of infinite size should be used which is practically impossible. The simple solution to this problem is to use number of large lengths, (say $L = \{L_1, L_2, \ldots L_n\}$, where n is a finite number and $L_1 < L_2 < \ldots < L_n$), and extrapolate the results for infinite lattice. The visual structure of the square lattice is as follows 4.11. This is and empty lattice structure. Filled circles are for occupied site and filled bonds are for occupied bonds 4.12.

4.9.6 Site Percolation

The algorithm for site percolation is as follows,

- 1. take a square lattice of length L.
- 2. fill all $2L^2$ bonds initially.
- 3. occupy a randomly chosen site and it will join some clusters.
- 4. each time a site is occupied, it will get connected to four neighboring bonds and will form a cluster of size 4. Note that we define cluster size by number of bonds in it.
- 5. if a site is occupied and right next to it there is another occupied site and a cluster of size 7 will be formed.

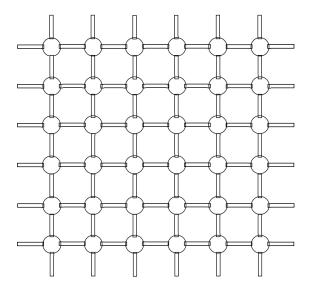


Fig. 4.11 Square Lattie (empty) of length 6



Fig. 4.12 Site and Bond symbol (empty and occupied).

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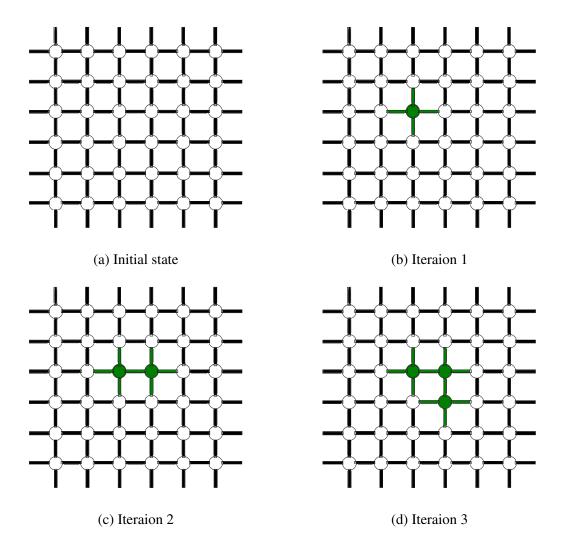


Fig. 4.13 Growth of a Cluster in Site Percolation on square Lattice

6. this process is repeated until all the sites are occupied and only one cluster remains

The formation of cluster is visualized in the figure 4.13.

4.9.7 Bond Percolation

The algorithm for bond percolation is as follows,

- 1. take a square lattice of length L.
- 2. fill all L^2 the sites initially.
- 3. occupy a randomly chosen bond and it will join some clusters.

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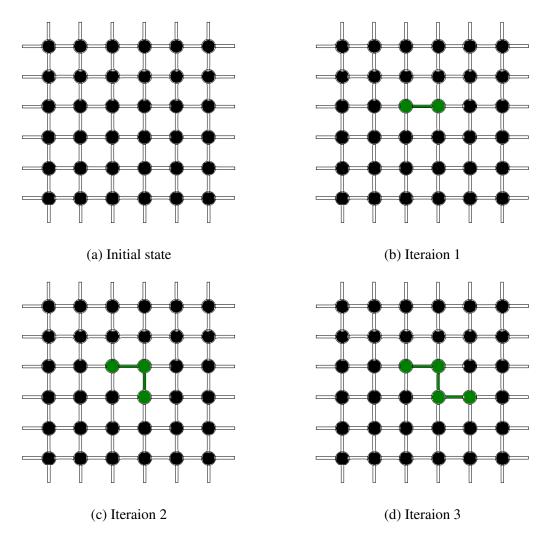


Fig. 4.14 Growth of a Cluster in Bond Percolation on square Lattice

- 4. each time a bond is occupied, it will get connected to two neighboring sites and will form a cluster of size 2. Here cluster size by number of sites in it.
- 5. if a bond is occupied and right next to it there is another occupied bond and they are connected by a site and a cluster of size 3 will be formed.
- 6. this process is repeated until all the bonds are occupied and only one cluster remains

The formation of cluster is visualized in the figure 4.14.

Chapter 5

Ballistic Deposition on Square Lattice

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 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 exponent τ which characterizes the cluster size distribution function $n_s(p_c) \sim s^{-\tau}$ 4.5.8 and the fractal dimension d_f that characterizes the spanning cluster at p_c 4.5.11. 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 exhist on RSBD.

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. 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 the main theme of this thesis.

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.

5.1 Site Percolation Redefined

5.2 Structure and Algorithm

Random percolation (RP) model can also be seen as a random sequential adsorption (RSA) 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) 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 neighour site along the same line to make room for itself. However, the trial attempt of pushing the neighbour is successful if the next neibhouring 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 primery 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 diposoted 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, ..., L, the second row again from left to right as i = L + 1, L + 2,, 2L and we continue this till we reach the bottom row which we label as $i = (L - 1)L + 1, ..., L^2$. Then at each step we pick a discrete random number R from $1, 2, ..., L^2 - 1, L^2$ 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 successul 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 ocupied too but the next nearest neighbour site is empty then the neighbour move to the empty site to make space for the incoming perticle to be deposited there.

- 1. take a square lattice of length L.
- 2. choose a site randomly
- 3. if the chosen site is empty then occupy it else choose one of the four neighbor randomly
- 4. if the chosen neighbor is empty then occupy it else choose second nearest neighbor in that direction
- 5. if the second nearest neighbor is empty then occupy the site else ignore this step

5.3 Finite Size Scaling in Percolation Theory

5.4 Finding Numerical Values

5.4.1 Critical occupation probability, p_c

When we occupy sites of the square lattice, initially, there are only cluster 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 the result of 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 5.1 shows the graph of the spanning probability, w(p,L), versus the occupation probability p for different interactions (L0,L1,L2) for different lengths. We have found that p_c is 0.5927,0.5782,0.5701 for L0,L1,L2 respectively. Thus for long range interaction p_c is smaller than for short range interaction. The quantity w(p,L) is called

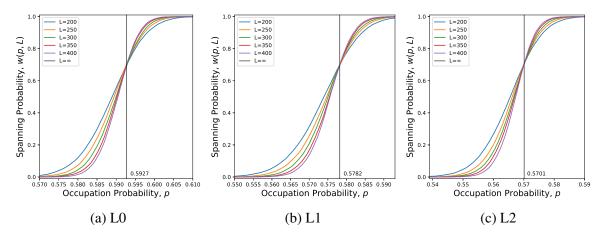


Fig. 5.1 Spanning Probability, w(p,L) vs Occupation Probability, p

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 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 got our critical point, p_c , as the intersection of the w(p,L) for different lengths.

5.4.2 Spanning Probability and finding 1/v

From the figure 5.1 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, say y = 0.1, 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. If we now use the finite size scaling (FSS) hypothesis

$$w = (p - p_c)L^{1/\nu} (5.1)$$

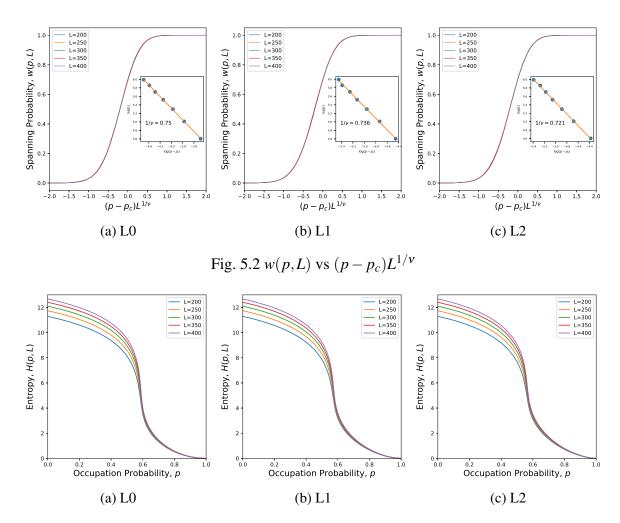


Fig. 5.3 Entropy, H(p,L) vs Occupation Probability, p

we get a very good data collapse for L0, L1, L2 and got 1/v as 0.75, 0.736, 0.721 respectively which is shown in figure 5.2. That is they are self-similar ??.

5.4.3 Entropy, Specific Heat and finding α

For any phase transition model the entropy is crucial. In percolation theory we use Shannon Entropy [78]. Using the definition \ref{figure} we get the figure 5.3 And since the specific heat C(p,L) is nothing but the derivative of entropy, by simply differentiating entropy we get the specific heat (although we need to perform convolution?? in order to get a smooth curve) shown in figure 5.4. 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/v obtained from 5.4.2 and get the graph as in figure \ref{figure} . From this graph we will not 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

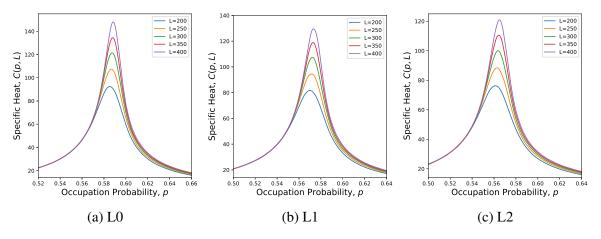
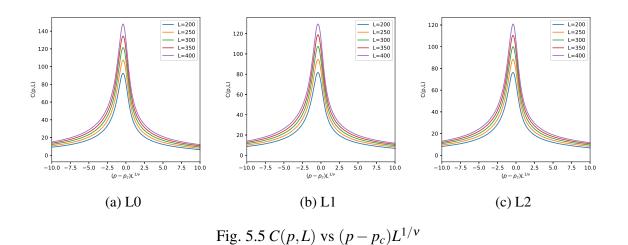


Fig. 5.4 Specific Heat, C(p,L) vs Occupation Probability, p



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 0.906,0.911,0.919 for L0,L1,L2 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 L0,L1,L2 and it is shown in figure 5.6

5.4.4 Order Parameter and finding β

Order parameter, also knows 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 ?? we obtain the order parameter for our system and it is shown in the figure 5.7. Since using spanning cluster and the largest cluster gives the same exponent, it really does not matter 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 in

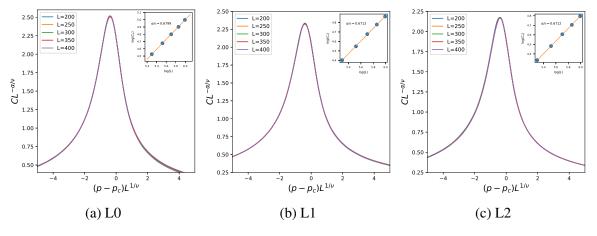


Fig. 5.6 $CL^{-\alpha/\nu}$ vs $(p-p_c)L^{1/\nu}$

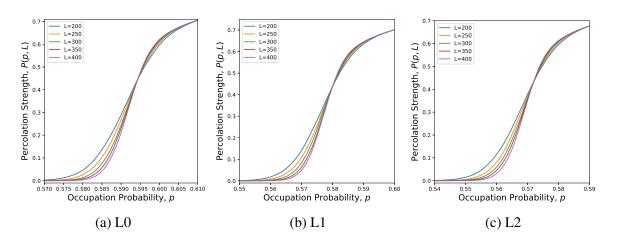


Fig. 5.7 Order Parameter, P(p,L) vs Occupation Probability, p

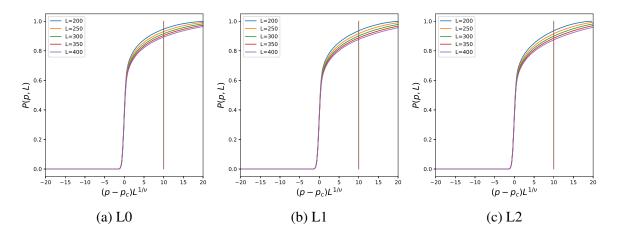


Fig. 5.8 Order Parameter, P(p,L) vs Occupation Probability, p

Fig. 5.9
$$P(p,L)$$
 vs $(p-p_c)L^{1/v}$

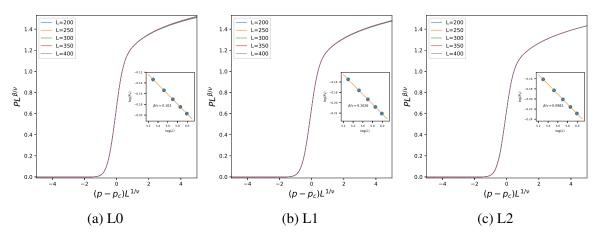


Fig. 5.10 $PL^{\beta/\nu}$ vs $(p - p_c)L^{1/\nu}$

section 5.4.2 we scale the *x*-values as $(p-p_c)L^{1/\nu}$ and get the following figure 5.8. Then in figure 5.8 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 5.10)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 5.10.

5.4.5 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 5.11. And if we scale the x values and plot χ vs $(p-p_c)L^{1/\nu}$ we get all the peak point

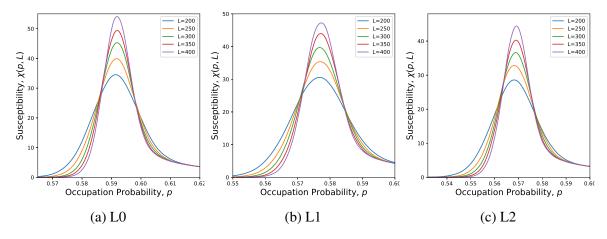
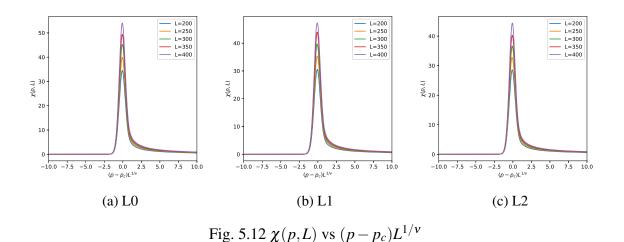


Fig. 5.11 Susceptibility, $\chi(p,L)$ vs Occupation Probability, p



aligned (figure 5.12). Note that the value of 1/v is known from section 5.4.2. 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/v . And using the FSS hypothesis we plot $\chi L^{-\gamma/v}$ vs $(p-p_c)L^{1/v}$ and obtain a perfect data collapse. It is shown in figure 5.13. We obtain the values of γ to be 0.8543,0.8542,0.882.

5.4.6 Cluster Size Distribution

 n_s vs s graph

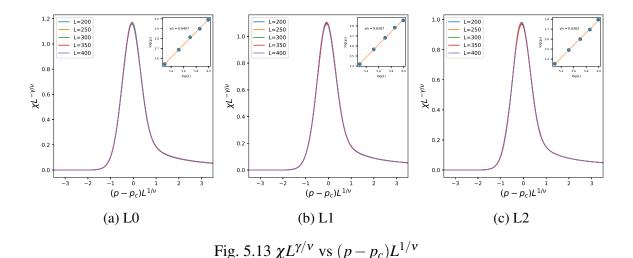


Fig. 5.14 Number of cluster of size s, n_s vs size of the cluster s

5.4.7 Cluster Rank Size Distribution

5.4.8 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 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

Fig. 5.15
$$\log(n_s)$$
 vs $\log(s)$

85

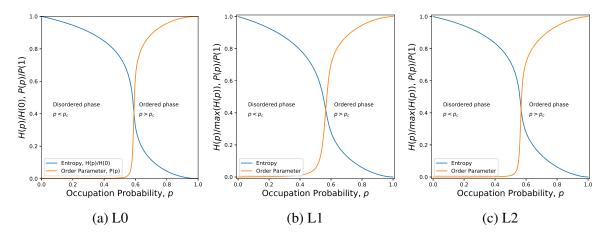


Fig. 5.16 H(p,L)/H(0,L) or P(p,L)/P(1,L) vs p

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 ?? containing both entropy and order parameter can show this process. We have normalized the entropy (figure 5.3) to match with the order parameter (figure 5.7).

5.4.9 Fractal Dimension

At critical point the square lattice shows the property of a fractal. A fractal 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. We use the relation

$$S \sim L^{d_f} \tag{5.2}$$

taking log we get

$$\log(S) = d_f \log(L) \tag{5.3}$$

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 L0, L1, L2 which is listed in 6.2.

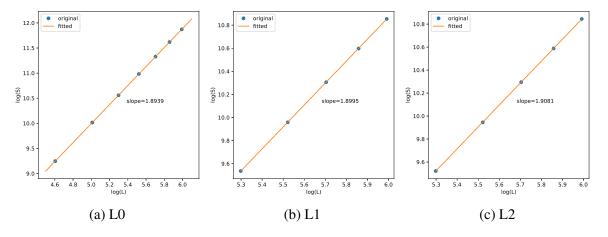


Fig. 5.17 $\log(S)$ vs $\log(L)$

Chapter 6

Summary and Discussion

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 , 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 exponent τ which characterizes the cluster size distribution ?? and 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 exhist on RSBD.

We denote L0, L1, L2 for expressing direct, first nearest neighbor and second nearest neighbor interaction respectively. Up until now we knew the exponents for L0 for old definition of site percolation. We have found same exponents for the thermodynamically consistent new definition of site percolation and we also have investigated for short and long range interactions and we call this L1 and L2 respectively. Note that L1 is the case where we can choose the first nearest neighbor and L2 is the case where we can chose 2nd nearest neighbor in the direction of first nearest neighbor. We can use new feature of L1 only if the feature of L0 is unavailable, i.e., the selected site is already occupied. Similarly we can use new feature of L2 only if the feature of L0 and L1 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.

The combined exponents are listed below

The critical exponents found in all cases are listed below,

Here we notice that the critical point decreases as we increase the range of interaction. But the fractal dimension increases. This is reasonable since my occupying nearest and

Interaction	p_c	1/v	α/ν	β/ν	γ/ν
L0	0.5927	0.75	0.6799	0.103	0.64071
L1	0.5782	0.736	0.6712	0.1026	0.6287
L2	0.5701	0.721	0.6631	0.0982	0.6362

Table 6.1 List of combined exponents

Interaction	p_c	1/v	α	β	γ	$\alpha + 2\beta + \gamma$	d_f
LO	0.5927	0.75	0.906	0.137	0.8543	2.0347	1.8939
L1	0.5782	0.736	0.911	0.139	0.8542	2.044	1.8994
L2	0.5701	0.721	0.919	0.136	0.882	2.07	1.90810

Table 6.2 List of exponents

second nearest neighbor we are increasing the change 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.

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Appendix A

Percolation

A.1 Algorithm

A.2 Code

A.2.1 Index

The index.h file

```
#ifndef SITEPERCOLATION_INDEX_H
    #define SITEPERCOLATION_INDEX_H
   #include <ostream>
   #include <iostream>
   #include <sstream>
   #include <vector>
   #include "../types.h"
   #include "../exception/exceptions.h"
   #include "../lattice/bond_type.h"
13
   struct Index {
    value_type row_{};
15
    value_type column_{};
   ~Index()
                                 = default;
    Index()
                                  = default;
    Index(value_type x, value_type y) : row_{x}, column_{y} {}
```

```
};
    class IndexRelative {
26
    public:
27
    int x_{};
28
    int y_{};
29
    ~IndexRelative()
                                              = default;
31
    IndexRelative()
                                              = default;
32
    IndexRelative(int x, int y) : x_{x} {x}, y_{y} {}
34
35
    };
36
37
38
    struct BondIndex {
39
    BondType bondType;
40
42
    value_type row_;
    value_type column_;
43
    ~BondIndex()
                                            = default;
45
    BondIndex()
                                            = default;
46
47
    BondIndex(BondType hv, value_type row, value_type column)
    : row_{row}, column_{column}
    bondType = hv;
51
52
53
    bool horizontal() const { return bondType == BondType:: Horizontal;}
54
    bool vertical() const { return bondType == BondType:: Vertical;}
55
    };
57
    std::ostream& operator <<(std::ostream& os, const Index& index);</pre>
    bool operator == (const Index& index1, const Index& index2);
60
    bool operator <(const Index& index1, const Index& index2);</pre>
61
    std::ostream& operator <<(std::ostream& os, const IndexRelative& index)
63
```

```
std::ostream& operator <<(std::ostream& os, const BondIndex& index);
    bool operator == (BondIndex index1, BondIndex index2);
    bool operator <(BondIndex index1, BondIndex index2);</pre>
68
69
    /**
70
   * Get 2nd nearest neightbor / sin the direction of 1st nearest
71
     neighbor, while @var center is the center
    */
72
    Index get_2nn_in_1nn_direction(Index center, Index nn_1, value_type
     length);
    std::vector<Index> get_2nn_s_in_1nn_s_direction(Index center, const
     std::vector<Index> &nn_1, value_type length);
75
    #endif //SITEPERCOLATION_INDEX_H
76
77
```

The **index.cpp** file

```
#include <iomanip>
    #include "index.h"
    using namespace std;
    ostream& operator << (ostream& os, const Index& index)
    return os <<'(' << index.row_ << ',' << index.column_ << ')';</pre>
10
    ostream& operator << (ostream& os, const IndexRelative& index)
11
    return os << '(' << std::setw(3) << index.x_ << ',' << std::setw(3) <<
13
      index.y_ << ')';
14
    }
    bool operator == (const Index& index1, const Index& index2) {
    return (index1.row_ == index2.row_) && (index1.column_ == index2.
17
     column_);
18
19
    bool operator < (const Index& index1, const Index& index2) {
    if (index1.row_ < index2.row_)</pre>
    return true;
22
    if (index1.row_ == index2.row_){
```

```
return index1.column_ < index2.column_;</pre>
26
    return false;
27
28
29
    ostream& operator << (ostream& os, const BondIndex& index) {
30
    if (index.horizontal()){
31
    // horizontal bond
    os << "<->";
34
    if (index.vertical()){
    // vertical bond
    os << "<|>";
37
38
    return os << '(' << index.row_ << ',' << index.column_ << ')';</pre>
39
41
    bool operator == (BondIndex index1, BondIndex index2) {
42
    if(index1.horizontal() == index2.horizontal() || index1.vertical() ==
        index2. vertical()){
    // horizontal or vertical
    return index1.row_ == index2.row_ && index1.column_ == index2.column_;
45
    return false;
47
48
    bool operator < (BondIndex index1, BondIndex index2) {
51
    cout << "not yet defined : line " << __LINE__ << endl;</pre>
52
    return false;
53
54
55
56
    * Get the 2nd nearest nearest neighbor in the direction of 1st nearest
       neighbor.
    * Periodicity is not considered here.
    * @param center
    * @param nn_1
61
    * @param length
    * @return
63
64
```

```
Index get_2nn_in_1nn_direction(Index center, Index nn_1, value_type
    int delta_c = int(nn_1.column_) - int(center.column_);
    int delta_r = int(nn_1.row_) - int(center.row_);
67
    if (delta_c == 0 \&\& delta_r == 0){
68
    cout << "Both indices are same : line " << __LINE__ << endl;</pre>
70
    else if (delta_c > 1 | l delta_r > 1){
71
    // meaning, the sites are on the opposite edges
              cout << "2nd index is not the First nearest neighbor: line
     " << __LINE__ << " : file " << __FILE__ << endl;
75
    return Index {(nn_1.row_ + delta_r + length) % length, (nn_1.column_ +
      delta_c + length) % length };
77
79
80
    * Get all second nearest neighbors based on the first nearest
      neighbors.
    * Periodicity is not considered here
82
    * @param center
83
    * @param nn_1
    * @param length
    * @return
    */
87
    vector < Index > get_2nn_s_in_1nn_s_direction (Index center, const vector <
     Index > &nn_1, value_type length){
    vector <Index > nn_2(nn_1.size());
    for(size_t i{}; i != nn_1.size() ; ++i){
91
    int delta_c = int(nn_1[i].column_) - int(center.column_);
92
    int delta_r = int(nn_1[i].row_) - int(center.row_);
93
    if (delta_c == 0 \&\& delta_r == 0){
    cout << "Both indices are same : line " << __LINE__ << endl;</pre>
95
    else if (delta_c > 1 | l | delta_r > 1)
    // meaning, the sites are on the opposite edges
    11
                   cout << "center " << center << " nn " << nn 1 << endl;
99
                   cout << "2nd index is not the First nearest neighbor:
100
     line " << __LINE__ << " : file " << __FILE__ << endl;
    }
101
```

A.2.2 Site and Bond

The **site.h** file

```
#ifndef SITEPERCOLATION_SITE_H
    #define SITEPERCOLATION_SITE_H
   #include <array>
   #include <set>
   #include <vector>
   #include <iostream>
   #include <memory>
   #include "../index/index.h"
11
   #include "../types.h"
12
13
    /**
15
    * single Site of a lattice
    */
    struct Site {
   /**
20
   * if true -> site is placed.
   * if false -> the (empty) position is there but the site is not (
    required for site percolation)
    */
    bool _status{false};
    int _group_id\{-1\};
    Index _id{};
26
    value_type _weight{}; // when one site is occupied multiple times
    only weight increases by occupation
28
    //relative distance from the root site. \{0,0\} if it is the root site
29
  //very useful for detecting wrapping // todo
```

```
IndexRelative _relative_index {0,0};
          std::vector<Index> _neighbor{};
    // _connection[0] -> _connection between "set_ID" and "_neighbor[0]"
34
    /**
36
    * using set gives following advantages
37
    * 1. Keeps elements sorted
    * 2. automatically manage repeated value
    */
    //
          std::set<int> _connection{};
    public:
43
44
    ~Site()
                             = default;
45
    Site()
                             = default;
46
    Site (const Site &)
                                    = default;
    Site (Site & & )
                            = default;
48
    Site& operator = (const Site&) = default;
    Site& operator = (Site&&) = default;
    Site(Index id, value_type length){
52
    // I have handle _neighbor or corner points and edge points carefully
53
    if (id.row_ >= length || id.column_ >= length){
    std::cout << "out of range : line " << __LINE__ << std::endl;
55
56
    _{id.row} = id.row_{;}
57
    _id.column_ = id.column_;
              _neighbor = Lattice_Helper::get_neighbor(id, length);
    //
61
62
    bool isActive() const { return _status;}
63
    void activate(){ _status = true;}
64
    void deactivate() {
    _{relative\_index} = \{0,0\};
    _{group\_id} = -1;
    _status = false;
    Index ID() const { return _id;}
70
71
    * Group get_ID is the set_ID of the cluster they are in
72
    */
73
    int get_groupID() const {return _group_id;}
```

```
void
              set_groupID(int g_id) {_group_id = g_id;}
     std::stringstream getSite() const {
     std::stringstream ss;
78
     if (is Active ())
79
     ss \ll id;
     else
81
     ss << "(*)";
82
     return ss;
83
     value_type weight() const {return _weight;}
     void increaseWeight() { _weight += 1;}
87
88
     void relativeIndex(IndexRelative r){
89
     _relative_index = r;
90
     }
91
92
     void relativeIndex(int x, int y){
93
     _{relative\_index} = \{x, y\};
95
96
     IndexRelative relativeIndex() const {return _relative_index;}
97
98
     };
99
100
     std::ostream& operator <<(std::ostream& os, const Site& site);
101
     bool operator == (Site& site1, Site& site2);
    #endif //SITEPERCOLATION_SITE_H
104
105
```

file: site.cpp

```
#include <iomanip>
#include "site.h"

std::ostream& operator <<(std::ostream& os, const Site& site)

{
    if(site.isActive())
    return os << site._id;
    else
    return os << "(*)";
}</pre>
```

file: bond_type.h

```
#ifndef PERCOLATION_BOND_V2_H

#define PERCOLATION_BOND_V2_H

/**

* Only two type bonds in 2D lattice

*/

enum class BondType{

Horizontal,

Vertical

};

#endif //PERCOLATION_BOND_V2_H
```

file: bond.h

```
#ifndef SITEPERCOLATION_BOND_H
   #define SITEPERCOLATION_BOND_H
   #include <ostream>
   #include <iostream>
   #include <sstream>
   #include "../index/index.h"
   #include "../types.h"
   /**
11
   * A bond has two end
   * say a 5x5 lattice bond between end1 (0,0) and end2 (0,1)
   * if _status is false -> bond is not there
14
15
   */
16
   struct Bond{
   // check if active or not
bool _status{false};
```

```
value_type _length;
    int _{group_id}\{-1\};
    BondType bondType;
23
    //relative distance from the root site. \{0,0\} if it is the root site
24
    //very useful for detecting wrapping // todo
25
    IndexRelative _relative_index {0,0};
26
28
    Index _end1;
    Index _end2;
    BondIndex _id;
32
33
    ~Bond() = default;
34
    Bond() = default;
35
    Bond(Index end1, Index end2, value_type length){
    _end1.row_ = end1.row_;
37
    _end1.column_ = end1.column_;
    _end2.row_ = end2.row_;
    _end2.column_ = end2.column_;
40
41
    // correct the bond here
42
    _length = length;
43
    // check if the bond is valid??
44
    if (_end1.row_ == _end2.row_){
45
    bondType = BondType::Horizontal;
                  horizontal = true;
    // means x_ values are equal
    if (_end1.column_ > _end2.column_){
    // case (0,0) < -> (0,4) for L=5 and
    // case (0,4) < -> (0,0) are equal for bond like this end1=(0,4) end2
51
    // for all other cases lower index is end1
    if(\_end1.column\_ == \_length -1 \&\& \_end2.column\_ ==0){
    // do nothing
54
                            std :: cout << "_end1.y_ == _length -1 && _end2.y_
    //
     ==0 : line " << __LINE__ << std::endl;
56
    else {
57
    // sort them out
    _end1.column_ = end2.column_;
59
    _end2.column_ = end1.column_;
60
61
```

```
else if (_end1.column_ < _end2.column_){</pre>
     if(\_end1.column\_ == 0 \&\& \_end2.column\_ == \_length -1)
     _end1.column_ = end2.column_;
65
     _end2.column_ = end1.column_;
     }
     11
                     _{id} = set_{ID} < 3 > (\{0, _{end1.x_{,}}, _{end1.y_{,}});
70
     else if(_end1.column_ == _end2.column_){
     bondType = BondType:: Vertical;
     //
                     vertical = true;
     // means y_ values are equal
74
     if (_end1.row_ > _end2.row_){
75
     // case (0,0) < -> (4,0) for L=5 and
     // case (4,0) < -> (0,0) are equal for bond like this end1=(4,0) end2
     =(0,0)
     // for all other cases lower index is end1
     if(\_end1.row\_ == \_length -1 \&\& \_end2.row\_ ==0){
     // do nothind
                              std :: cout << "_end1.x_ == _length -1 && _end2.x_
      ==0 : line " << __LINE__ << std::endl;
82
     else {
83
     // sort them out
     _end1.row_ = end2.row_;
     _end2.row_ = end1.row_;
     else if(_end1.row_ < _end2.row_){</pre>
     if(\_end1.row\_ == 0 \&\& \_end2.row\_ == \_length - 1){
     _end1.row_ = end2.row_;
91
     _end2.row_ = end1.row_;
93
     //
                     _{id} = set_{ID} < 3 > (\{1, _{end1.x_{,}} end1.y_{,}\});
95
     std::cout << '(' << _end1.row_ << ',' << _end1.column_ << ')' << "<->"
    << '(' << _end2.row_ << ',' << _end2.column_ << ')'</pre>
     << " is not a valid bond : line " << __LINE__ << std :: endl;
100
     //
                    _{id} = set_{ID} < 3 > (\{-1, -1, -1\});
101
     }
102
103
```

```
_{id} = \{(horizontal) ? Oul : 1ul, _end1.x_, end1.y_\}; //
      unsigned long
    _id = BondIndex(bondType, _end1.row_, _end1.column_); // unsigned
105
      long
106
     }
107
108
     std::vector < Index > getSites() const { return {_end1, _end2};}
109
110
     Index id() const {
111
     return _end1;
114
     BondIndex ID() const {
     return _id;
116
118
     void activate() { _status = true;}
119
     void deactivate() {
120
     _{relative\_index} = \{0,0\};
121
     _{group\_id} = -1;
     _status = false;
124
     bool isActive() const { return _status;}
125
126
     * Group get_ID is the set_ID of the cluster they are in
127
128
     int get_groupID() const {return _group_id;}
     void set_groupID(int g_id) { _group_id = g_id;}
130
132
     std::stringstream getBondString() const {
     std::stringstream ss;
134
     if (isActive()) {
     // place '-' for horizontal bond and 'l' for vertical bong
136
     if (bondType == BondType:: Horizontal) {
137
     ss << '(' << _end1 << "<->" << _end2 << ')';
138
     }
     else {
140
     ss << '(' << _end1 << "<|>" << _end2 << ')';
141
142
     }
143
     e1se
144
    ss << "(**)";
145
```

```
return ss;
     bool isHorizontal() const { return bondType == BondType :: Horizontal;}
149
     bool is Vertical() const { return bondType == BondType :: Vertical;}
150
151
     void relativeIndex(IndexRelative r){
152
     _relative_index = r;
153
     }
154
     void relativeIndex(int x, int y){
     _{relative\_index} = \{x,y\};
157
158
159
     IndexRelative relativeIndex() const {return _relative_index;}
160
     };
161
162
163
                      operator <<(std::ostream& os, const Bond& bond);
     std::ostream&
     bool
                      operator == (Bond a, Bond b);
                      operator < (const Bond& bond1, const Bond& bond2);
     bool
166
                      operator > (const Bond& bond1, const Bond& bond2);
     bool
167
168
169
     #endif //SITEPERCOLATION_BOND_H
170
171
```

file: bond.cpp

```
#include "bond.h"
3
      * use '-' and '|' in between '<>' to indicate horizontal or vertical
      bond
      * ((0,1) < -> (0,0)) for horizontal bond
      * ((1,1) < | > (0,1)) for vertical bond
      * @param os
      * @param bond
      * @return
      */
10
      std::ostream& operator <<(std::ostream& os, const Bond& bond)
11
12
      if (bond.isActive()) {
13
      // place '-' for horizontal bond and 'l' for vertical bong
```

```
if (bond.is Horizontal()) {
      return os << '(' << bond._end1 << "<->" << bond._end2 << ')';</pre>
      return os << '(' << bond. end1 << "<|>" << bond. end2 << ')';
18
19
      e1se
20
      return os << "(**)";
22
      bool operator == (Bond a, Bond b)
      if(a.isHorizontal() && b.isHorizontal())
27
      return (a.id().row_ == b.id().row_) && (a.id().column_ == b.id().
     column_);
29
      if(a.isVertical() && b.isVertical()){
30
      return (a.id().row_ == b.id().row_) && (a.id().column_ == b.id().
31
     column_);
      }
      return false;
34
      }
35
             operator < (const Bond& bond1, const Bond& bond2) {
37
      if(bond1.isHorizontal() && bond2.isHorizontal()){
      return bond1._end1.column_ < bond2._end1.column_;</pre>
39
      if (bond1.is Vertical() && bond2.is Vertical()){
      return bond1._end1.row_ < bond2._end1.row_;</pre>
42
43
      return bond1.isHorizontal();
44
      }
45
46
             operator > (const Bond& bond1, const Bond& bond2) {
      if (bond1.isHorizontal() && bond2.isHorizontal()){
      return bond1._end1.column_ > bond2._end1.column_;
51
      if (bond1.is Vertical() && bond2.is Vertical()){
52
      return bond1._end1.row_ > bond2._end1.row_;
53
54
      return bond1.isVertical();
55
56
```

57

A.2.3 Lattice

file: lattice.h

```
#ifndef SITEPERCOLATION_LATTICE_H
   #define SITEPERCOLATION_LATTICE_H
   #include <vector>
   #include <cmath>
   #include "../percolation/cluster.h"
   #include "../types.h"
   #include "site.h"
   #include "bond.h"
13
   /**
   * The square Lattice
    * Site and Bonds are always present But they will not be counted
    unless they are activated
   * always return by references, so that values in the class itself is
     modified
    */
    class SqLattice {
19
         std::vector<std::vector<Index>> _clusters; // only store index
    in the cluster
    std::vector<std::vector<Site>> _sites; // holds all the sites
    std::vector < std::vector < Bond>> _h_bonds; // holds all horizontal
    std::vector<std::vector<Bond>> _v_bonds; // holds all vertical bonds
23
24
    bool _bond_resetting_flag=true; // so that we can reset all bonds
25
    bool _site_resetting_flag=true; // and all sites
    value_type _length { };
    private:
30
    void reset_sites();
31
    void reset_bonds();
    public:
33
~SqLattice() = default;
```

```
SqLattice() = default;
    SqLattice (SqLattice &) = default;
    SqLattice (SqLattice&&) = default;
    SqLattice& operator=(const SqLattice&) = default;
38
    SqLattice& operator = (SqLattice&&) = default;
39
40
    SqLattice(value_type length, bool activate_bonds, bool activate_sites,
41
      bool bond_reset, bool site_reset);
42
    void reset(bool reset_all=false);
    /* **************
46
    * I/O functions
47
   *****************************
48
   void view_sites();
49
   void view_sites_extended();
   void view_sites_by_id();
51
   void view_sites_by_relative_index();
   void view_bonds_by_relative_index();
   void view_bonds_by_relative_index_v2();
   void view_bonds_by_relative_index_v3();
55
   void view_bonds_by_relative_index_v4();
56
   void view_by_relative_index();
57
   void view(); // view lattice bonds and sites together
58
59
   void view_h_bonds();
   void view_v_bonds();
62
   void view_bonds(){
   view_h_bonds();
   view_v_bonds();
65
66
67
   void view_h_bonds_extended();
   void view_v_bonds_extended();
   void view_bonds_by_id();
71
73
   /* *************
   * Activation functions
74
    *************
75
   void activateAllSite();
76
   void activateAllBond();
77
```

```
void activate_site(Index index);
    void activateBond(BondIndex bond);
    void deactivate site(Index index);
81
    void deactivate_bond(Bond bond);
82
84
    value_type length() const { return _length;}
85
    //
           Site getSite(Index index);
    //
           Bond get_h_bond(Index set_ID);
    //
           Bond get_v_bond(Index set_ID);
90
    Site& getSite(Index index);
91
           Site&& getSiteR(Index index);
    //
92
    Bond& get_h_bond(Index id);
93
    Bond& get_v_bond(Index id);
    Bond& getBond(BondIndex);
95
    const Site& getSite(Index index) const ;
    void setGroupID(Index index, int group_id);
99
    void setGroupID(BondIndex index, int group_id);
100
    int getGroupID(Index index);
101
    int getGroupID(BondIndex index);
102
103
104
    /*
    * Get Neighbor from given index
106
107
                                                                               ******
      */
    std::vector<Index> get_neighbor_site_indices(Index site); // site
108
      neighbor of site
    std::vector<BondIndex> get_neighbor_bond_indices(BondIndex site); //
      bond neighbor of bond
    std::vector<Index> get_neighbor_indices(BondIndex bond);
                                                                   // two site
110
       neighbor of bond.
    static std::vector<Index> get_neighbor_site_indices(size_t length,
112
      Index site); // 4 site neighbor of site
```

file: lattice.cpp

```
#include <iomanip>
    #include "lattice.h"
    #include "../ util/printer.h"
    using namespace std;
    /**
                      -> length of the lattice
    * @param length
10
    * @param activate_bonds -> if true all bonds are activated by default
11
                                and will not be deactivated as long as the
     object exists,
                                even if SLattice::reset function is called.
13
    * @param activate_sites -> if true all sites are activated by default
14
                                and will not be deactivated as long as the
15
    object exists,
                               even if SLattice::reset function is called.
16
    */
17
    SqLattice::SqLattice(
    value_type length,
    bool activate_bonds, bool activate_sites,
    bool bond_reset, bool site_reset)
21
    : _length { length }, _bond_resetting_flag { bond_reset },
22
     _site_resetting_flag { site_reset }
23
    cout << "Constructing Lattice object : line " << __LINE__ << endl;</pre>
    _sites = std::vector<std::vector<Site>>(_length);
25
    _h_bonds = std::vector<std::vector<Bond>>(_length);
    _v_bonds = std::vector<std::vector<Bond>>(_length);
```

```
if (!activate_bonds && !activate_sites) {      // both are deactivated by
    for (value_type i{}; i != _length; ++i) {
29
    _sites[i] = std::vector < Site > (_length);
30
    _h\_bonds[i] = std::vector < Bond > (_length);
31
    _v_bonds[i] = std::vector < Bond > (_length);
32
    for (value_type j{}; j != _length; ++j) {
33
    _sites[i][j] = Site(Index(i, j), _length);
    _{h\_bonds[i][j]} = \{Index(i, j), Index(i, (j + 1) \% _length), _length\};
35
    v\_bonds[i][j] = \{Index(i, j), Index((i + 1) \% \_length, j), \_length\};
    }
38
39
    else if(activate_bonds && !activate_sites) {
                                                        // all bonds are
40
      activated by default
    for (value_type i{}; i != _length; ++i) {
41
    _sites[i] = std::vector < Site > (_length);
    _h\_bonds[i] = std::vector < Bond > (_length);
43
    _{v\_bonds[i]} = std:: vector < Bond > (_length);
    for (value_type j{}; j != _length; ++j) {
    \_sites[i][j] = Site(Index(i, j), \_length);
46
    _{h\_bonds[i][j]} = \{Index(i, j), Index(i, (j + 1) \% _length), _length\};
47
    v_{\text{bonds}}[i][j] = \{Index(i, j), Index((i + 1) \% length, j), length\};
48
    _h_bonds[i][j].activate();
    _v_bonds[i][j].activate();
50
    }
    }
52
53
    else if(!activate_bonds && activate_sites) {      // all sites are
      activated by default
    for (value_type i{}; i != _length; ++i) {
55
    _sites[i] = std::vector < Site > (_length);
    _h\_bonds[i] = std::vector < Bond > (_length);
57
    _{v\_bonds[i]} = std:: vector < Bond > (_length);
58
    for (value_type j{}; j != _length; ++j) {
    \_sites[i][j] = Site(Index(i, j), \_length);
    _sites[i][j].activate();
    _{h\_bonds[i][j]} = {Index(i, j), Index(i, (j + 1) % _length), _length};
62
    v\_bonds[i][j] = \{Index(i, j), Index((i + 1) \% \_length, j), \_length\};
63
    }
64
    }
65
   else {
```

```
for (value_type i{}; i != _length; ++i) { // all bonds and sites are
       activated by default
    _sites[i] = std::vector < Site > (_length);
    _h_bonds[i] = std::vector < Bond>(_length);
70
    _v_bonds[i] = std::vector < Bond > (_length);
71
    for (value_type j{}; j != _length; ++j) {
72
    _sites[i][j] = Site(Index(i, j), _length);
73
    _sites[i][j].activate();
74
    _{h\_bonds[i][j]} = \{Index(i, j), Index(i, (j + 1) \% _length), _length\};
75
    _{v\_bonds[i][j]} = \{Index(i, j), Index((i + 1) \% _length, j), _length\};
    _h_bonds[i][j].activate();
77
    _v_bonds[i][j].activate();
78
    }
80
81
82
83
84
85
    * Activation and Deactivation
    *************************
    void SqLattice::activateAllSite()
88
    {
89
    for(value_type i{} ; i != _length ; ++i) {
90
    for (value_type j{}; j != _length; ++j) {
91
    _sites[i][j].activate();
92
93
    /**
98
    */
99
    void SqLattice::activateAllBond()
100
101
    for(value_type i{} ; i != _length ; ++i) {
102
    for (value_type j{}; j != _length; ++j) {
    _h_bonds[i][j].activate();
    _v_bonds[i][j].activate();
105
    }
106
    }
107
108
109
    void SqLattice::activate_site(Index index) {
```

```
cout << "activating site " << index << endl;</pre>
    _sites[index.row_][index.column_].activate();
114
    void SqLattice::activateBond(BondIndex bond) {
116
    // check if the bond is vertical or horizontal
    // then call appropriate function to activate _h_bond or _v_bond
118
    if(bond.horizontal()){ // horizontal
119
    if (_h_bonds[bond.row_][bond.column_].isActive()){
    cout << "Bond is already activated : line " << __LINE__ << endl;</pre>
    _h_bonds[bond.row_][bond.column_].activate();
124
    else if (bond. vertical()) // vertical
125
126
    if (_v_bonds[bond.row_][bond.column_].isActive()){
    cout << "Bond is already activated : line " << __LINE__ << endl;</pre>
128
    _v_bonds[bond.row_][bond.column_].activate();
130
131
    else {
    cout << bond << " is not a valid bond : line " << __LINE__ << endl;</pre>
    }
134
135
136
138
    void SqLattice::deactivate_site(Index index){
139
     _sites[index.row_][index.column_].deactivate();
140
    }
141
142
143
    void SqLattice::deactivate_bond(Bond bond) {
144
    // check if the bond is vertical or horizontal
    // then call appropriate function to activate _h_bond or _v_bond
    if (bond.is Horizontal()){
    if (_h_bonds[bond.id().row_][bond.id().column_].isActive()){
    cout << "Bond is already activated : line " << __LINE__ << endl;</pre>
149
150
     _h_bonds[bond.id().row_][bond.id().column_].deactivate();
151
152
    else if (bond.is Vertical())
153
```

```
if (_v_bonds[bond.id().row_][bond.id().column_].isActive()){
     cout << "Bond is already activated : line " << __LINE__ << endl;
    _v_bonds[bond.id().row_][bond.id().column_].deactivate();
158
159
    else {
160
    bond.activate();
161
     cout << bond << " is not a valid bond : line " << __LINE__ << endl;
162
163
167
    * Viewing methods
168
     *******************
169
170
     * View the sites of the lattice
    * place (*) if the site is not active
172
173
     */
    void SqLattice::view_sites()
175
    std::cout << "view sites" << std::endl;
176
     std::cout << '{';
177
     for(value_type i{} ; i != _length ; ++i) {
178
    if (i!=0) std::cout << " ";</pre>
179
    else std::cout << '{';</pre>
180
     for (value_type j{}; j != _length; ++j) {
    if (_sites[i][j]. isActive()){
    std::cout << _sites[i][j] ;</pre>
184
    else {
185
    std::cout << "(*)";
186
187
    if(j != _length -1)
188
    std::cout << ',';
189
190
     std::cout << '}';
191
    if(i != _length -1)
     std::cout << std::endl;</pre>
193
194
     std::cout << '}';
195
     std::cout << std::endl;</pre>
196
197
198
```

```
/**
199
     * View the sites of the lattice
        place (*) if the site is not active
       Shows the group_id along with sites
202
203
     * Very good output format. Up to lattice size < 100
204
205
     void SqLattice:: view_sites_extended()
206
207
     std::cout << "view sites" << std::endl;</pre>
     std::cout << '{';
     for(value_type i{} ; i != _length ; ++i) {
     if (i!=0) std::cout << " ";</pre>
211
     else std::cout << '{';</pre>
212
     for (value_type j{}; j != _length; ++j) {
213
     std::cout << std::setw(3) << _sites[i][j].get_groupID() << ":";
214
215
     if (_sites[i][j].isActive()) {
216
     cout << '(' << std::setw(2) << _sites[i][j]._id.row_ << ','</pre>
     << std::setw(2) << _sites[i][j]._id.column_ << ')';
219
     else {
220
     cout << std::setw(7) << "(*)";
     }
222
     if(j != _length -1)
224
     std::cout << ',';
225
     std::cout << '}';
227
     if(i != _length -1)
     std::cout << std::endl;</pre>
229
230
     std::cout << '}';
231
     std::cout << std::endl;</pre>
232
234
     /**
     * Displays group ids of sites in a matrix form
238
239
     void SqLattice::view_sites_by_id() {
240
     std::cout << "Sites by id : line " << __LINE__ << endl;
241
     cout << " ";
```

```
for(value_type j{}; j != _length; ++ j){
     cout << " " << setw(3) << j;
     cout << endl << " | ";
246
     for(value_type j{}; j != _length; ++ j){
247
     cout << "_ _ ";
248
249
     cout << endl;
250
     for(value_type i{} ; i != _length; ++i){
251
     cout << setw(3) << i << "|";
     for(value\_type j\{\} ; j != \_length ; ++ j)\{
     cout << setw(3) << _sites[i][j].get_groupID() << ' ';</pre>
255
     cout << endl;
256
257
258
259
     /**
263
     void SqLattice::view_sites_by_relative_index(){
264
     std::cout << "Relative index : line " << __LINE__ << endl;
265
     cout << "Format: \backslash" id (x,y)\backslash"" << endl;
266
     cout << " | ";
267
     for(value_type j{}; j != _length; ++ j){
268
     cout \ll setw(4) \ll j \ll 
     cout << endl;</pre>
271
     print_h_barrier(_length , "___|_" , "_____|_");
272
     for(value_type i{} ; i != _length; ++i){
273
     cout << setw(3) << i << "|";
274
     for(value_type j{} ; j != _length ; ++ j){
275
     if(sites[i][j].get_groupID() == -1)
276
     // left blank
277
                                                                     |";
     cout << setw(4) << _sites[i][j].get_groupID() << "</pre>
278
     continue;
     cout << setw(4) << _sites[i][j].get_groupID() << _sites[i][j].</pre>
281
      relativeIndex() << "|";
282
     cout << endl;
283
     print_h_barrier(_length , "___|_", "_____|_");
284
285
```

```
//
          print_h_barrier(_length , "___|_", "_____|_");
    }
    /**
289
    * View bonds in the lattice by relative index.
290
    * format : id(relative_index)
292
    void SqLattice::view_bonds_by_relative_index() {
293
294
    std::cout << "Bonds by id : line " << __LINE__ << endl;
    // printing indices for columns
    std::cout << " | ";
    for(value_type i{}; i != _length; ++i){
298
                                                 1 ":
    std::cout << " " << setw(4) << i << "
299
300
    std::cout << std::endl;</pre>
301
    // pringing H,V label
303
    print_h_barrier(_length , "____|_", "_____|_");
306
307
    // for each row there will be two columns
308
    for(value_type i{}; i != _length; ++i){
309
    std::cout << i << ' ';
310
    std::cout << "H |";
311
    for(value_type j1{}; j1 != _length; ++j1){
312
    std::cout << " < std::setw(3) << h_bonds[i][j1].get_groupID()
    << _h_bonds[i][j1].relativeIndex() << "|";</pre>
314
    std::cout << std::endl;
316
    | "); // just for
317
     better viewing
    std::cout << " " << "V | ";
318
    for(value_type j2{}; j2 != _length; ++j2){
319
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID()
320
    << _v_bonds[i][j2].relativeIndex() << " | ";
322
    std::cout << std::endl;</pre>
323
324
    // printing horizontal separator
325
    print_h_barrier(_length , "____|_", "_____|_");
326
327
    std::cout << std::endl;</pre>
```

```
332
    * View bonds in the lattice by relative index. id of the site is
333
    * format : id for site or id(relative_index) for bond
334
335
    void SqLattice::view_bonds_by_relative_index_v2() {
336
    std::cout << "Bonds by id: line " << __LINE__ << endl;
    cout << "site id -1 means isolated site and 0 means connected site in
    bond percolation(definition)" << endl;</pre>
    print_h_barrier(15, "_", "___", "_\n");
340
    cout << "|(site id) (horizontal bond id(relative index))|" << endl;</pre>
341
                                                  |" << end1;
    cout << "|( vertical bond id(relative index))</pre>
342
    print_h_barrier(15, "-", "---", "-\n");
343
    // printing indices for columns
344
    std::cout << " | ";
345
    for(value_type i{}; i != _length; ++i){
    std::cout << i << "
348
    std::cout << std::endl;
349
350
    // pringing H,V label
351
352
    353
    print_h_barrier(_length, "____|__", "______|___|);
    // for each row there will be two columns
    for(value_type i{}; i != _length; ++i){
357
    std::cout << i << ' ';
358
    std::cout << "H |";
359
    for(value_type j1{}; j1 != _length; ++j1){
360
    std::cout << std::setw(3) << _sites[i][j1].get_groupID();
    std::cout << " < std::setw(3) << _h_bonds[i][j1].get_groupID()
    << _h_bonds[i][j1].relativeIndex() << "|";</pre>
    std::cout << std::endl;</pre>
365
    | "); // just
366
     to see a better view
    std::cout << " " << "V | ";
367
    for(value_type j2{}; j2 != _length; ++j2){
368
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID()
369
```

```
<< _v_bonds[i][j2].relativeIndex() << "</pre>
372
    std::cout << std::endl;
373
    // printing horizontal separator
374
    print_h_barrier(_length , "____|__", "______|___|);
375
376
377
    std::cout << std::endl;</pre>
378
382
    * View bonds in the lattice by relative index. id of the site is
383
     showed
    * format : id(relative index) for site and only id for bond
384
    void SqLattice::view_bonds_by_relative_index_v3() {
386
    std::cout << "Bonds by id: line " << __LINE__ << endl;
    // cout << "site id -1 means isolated site and 0 means connected site
     in bond percolation (definition) " << endl;
    print_h_barrier(15, "_", "___", "_\n");
390
    cout << "|(site id) (horizontal bond id(relative index))|" << endl;</pre>
391
    cout << "|(vertical bond id(relative index))</pre>
                                                            |" << endl;
392
    print_h_barrier(15, "-", "---", "-\n");
393
    // printing indices for columns
394
    std::cout << " | ";
    for(value_type i{}; i != _length; ++i){
    std::cout << i << "
                                       1 ";
398
    std::cout << std::endl;</pre>
399
400
    // pringing H,V label
401
402
    403
    print_h_barrier(_length , "____|__", "______|___|);
    // for each row there will be two columns
    for(value_type i{}; i != _length; ++i){
407
    std::cout << i << ' ';
408
    std::cout << "H |";
409
    for(value_type j1{}; j1 != _length; ++j1){
```

```
std::cout << std::setw(3) << _sites[i][j1].get_groupID() << _sites[i][
     j1].relativeIndex();
    std::cout << " " << std::setw(3) << _h_bonds[i][j1].get_groupID() <<
      "|";
413
    std::cout << std::endl;
414
    | "); // just to
415
      see a better view
    std::cout << " " << "V | ";
416
    for(value_type j2{}; j2 != _length; ++j2){
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "
             1";
419
    std::cout << std::endl;
420
421
    // printing horizontal separator
422
    print_h_barrier(_length , "____|__", "______|___|);
423
424
425
    std::cout << std::endl;</pre>
427
428
429
    * View bonds in the lattice by relative index. id of the site is
430
     showed
    * format : id(relative index) for site and only id for bond
431
    * if any site is isolated relative index is not shown
432
    void SqLattice::view_bonds_by_relative_index_v4() {
    std::cout << "Bonds by id: line" << __LINE__ << endl;
436
    //cout << "site id -1 means isolated site and 0 means connected site
437
     in bond percolation (definition)" << endl;
    print_h_barrier(15, "_", "___", "_\n");
438
    cout << "|(site id) (horizontal bond id(relative index))|" << endl;</pre>
439
    cout << "|(vertical bond id(relative index))</pre>
                                                            |" << endl;
    print_h_barrier(15, "-", "---", "-\n");
    // printing indices for columns
    std::cout << " | ";
    for(value_type i{}; i != _length; ++i){
444
    std::cout << i << "
445
446
    std::cout << std::endl;</pre>
447
448
```

```
// pringing H,V label
    H | ");
    print_h_barrier(_length, "____|_", "_____|__");
452
453
    // for each row there will be two columns
454
    for(value_type i{}; i != _length; ++i){
455
    std::cout << i << ' ';
456
    std::cout << "H |";
457
    for(value_type j1{}; j1 != _length; ++j1){
    int id = _sites[i][j1].get_groupID();
    std::cout << std::setw(3) << id ;
    if (id != -1){
461
    cout << _sites[i][j1].relativeIndex();</pre>
462
    } else {
463
    cout << "(-,-) ";
464
    std::cout << " " << std::setw(3) << _h_bonds[i][j1].get_groupID() <<
      "|";
    std::cout << std::endl;
468
    | "); // just to
469
      see a better view
    std::cout << " " << "V | ";
470
    for (value_type j2 { }; j2 != _length; ++j2) {
471
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "
472
             1";
    std::cout << std::endl;</pre>
474
    // printing horizontal separator
476
    print_h_barrier(_length , "____|__", "______|___|);
477
478
479
    std::cout << std::endl;</pre>
481
485
    * View lattice (sites and bonds) by relative index.
486
    * format : id(relative_index)
487
    */
488
   void SqLattice::view_by_relative_index() {
```

```
490
    std::cout << "Bonds by id: line " << __LINE__ << endl;
    // printing indices for columns
    std::cout << " | ";
493
    for(value_type i{}; i != _length; ++i){
494
                                                  1 ":
    std::cout << i << "
495
496
    std::cout << std::endl;
497
    // pringing H,V label
    print_h_barrier(_length, " | ", " V
                                                                H ");
    print_h_barrier(_length , "____|__", "______
                                                               .____|;
502
503
    // for each row there will be two columns
504
    for(value_type i{}; i != _length; ++i){
505
    std::cout << i << ' ';
506
    std::cout << "H |";
507
    for(value_type j1{}; j1 != _length; ++j1){
508
    std::cout << std::setw(3) << _sites[i][j1].get_groupID() << _sites[i][
     j1].relativeIndex();
    std::cout << " " << std::setw(3) << _h_bonds[i][j1].get_groupID()
510
    << _h_bonds[i][j1].relativeIndex() << "|";</pre>
511
512
    std::cout << std::endl;
513
    ");
514
    // just to see a better view
    std::cout << " " << "V | ";
    for(value_type j2{}; j2 != _length; ++j2){
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID()
    << _v_bonds[i][j2].relativeIndex() << "</pre>
                                                          | | " ;
518
519
    std::cout << std::endl:
520
521
    // printing horizontal separator
    print_h_barrier(_length , "____|__" , "_____
523
524
    }
    //
             view_h_bonds_extended();
    // view v bonds extended();
527
    std::cout << std::endl;
528
529
    }
530
531
```

```
/**
532
    * View lattice (sites and bonds) by relative index.
    * format : id(relative_index)
535
    void SqLattice::view() {
536
537
    std::cout << "Bonds by id : line " << __LINE__ << endl;
538
    cout << "Structure " << endl;</pre>
539
    print_h_barrier(10, "_", "___", "_\n");
540
    cout << "|(site id) (horizontal bond id)|" << endl;</pre>
    cout << "|( vertical bond id) | " << endl;</pre>
    print_h_barrier(10, "-", "---", "-\n");
    // printing indices for columns
544
    std::cout << " | ";
545
    for(value_type i{}; i != _length; ++i){
546
    std::cout << i << " | ";
547
    std::cout << std::endl;</pre>
549
    // pringing H,V label
551
552
    553
    print_h_barrier(_length , "____|__", "_____|__");
554
555
    // for each row there will be two columns
556
    for(value_type i{}; i != _length; ++i){
557
    std::cout << i << ' ';
558
    std::cout << "H |";
    for(value_type j1{}; j1 != _length; ++j1){
    std::cout << std::setw(3) << _sites[i][j1].get_groupID();
    std::cout << " " << std::setw(3) << _h_bonds[i][j1].get_groupID() <<
562
     "|";
563
    std::cout << std::endl;</pre>
564
    print_h_barrier(_length , " | ", " | "); // just to see a
     better view
    std::cout << " " << "V | ";
    for (value_type j2 { }; j2 != _length; ++j2) {
    std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "
568
     ;
569
    std::cout << std::endl;</pre>
570
571
   // printing horizontal separator
```

```
print_h_barrier(_length , "____|__", "_____|__");
573
574
                 view h bonds extended();
     //
576
     //
                 view_v_bonds_extended();
577
     std::cout << std::endl;</pre>
578
579
     }
580
581
     /**
     */
585
     void SqLattice::view_h_bonds()
586
587
     std::cout << "view horizontal bonds" << std::endl;</pre>
588
     std::cout << '{';
589
     for(value_type i{} ; i != _length ; ++i) {
590
     if (i!=0) std::cout << " ";</pre>
591
     else std::cout << '{';</pre>
     for (value_type j{}; j != _length; ++j) {
593
     std::cout << _h_bonds[i][j] ;
594
     if(j != _length -1)
595
     std::cout << ',';
596
597
     std::cout << '}';
598
     if(i != _length -1)
599
     std::cout << std::endl;</pre>
     std::cout << '}';
602
     std::cout << std::endl;</pre>
603
604
605
     /**
606
607
     */
     void SqLattice::view_v_bonds()
     std::cout << "view vertical bonds" << std::endl;</pre>
611
     std::cout << '{';
612
     for(value_type i{} ; i != _length ; ++i) {
613
     if (i!=0) std::cout << " ";</pre>
614
     else std::cout << '{';</pre>
615
     for (value_type j{}; j != _length; ++j) {
616
```

```
std::cout << _v_bonds[i][j] ;</pre>
    if(j != _length -1)
619
    std::cout << ',';
620
    std::cout << '}';
621
    if(i != _length -1)
622
    std::cout << std::endl;</pre>
623
624
    std::cout << '}';
625
    std::cout << std::endl;</pre>
629
    /**
630
631
    */
632
    void SqLattice:: view_h_bonds_extended(){
633
    std::cout << "view horizontal bonds" << std::endl;</pre>
634
    std::cout << '{';
    for(value_type i{} ; i != _length ; ++i) {
    if (i!=0) std::cout << " ";
637
    else std::cout << '{';
638
    for (value_type j{}; j != _length; ++j) {
639
    640
     ][j] << ")";
    if(j != _length -1)
641
    std::cout << ',';
642
    std::cout << '}';
    if(i != _length -1)
    std::cout << std::endl;</pre>
646
647
    std::cout << '}';
648
    std::cout << std::endl;</pre>
649
    }
651
    /**
654
    void SqLattice::view_v_bonds_extended(){
655
    std::cout << "view vertical bonds" << std::endl;</pre>
656
    std::cout << '{';
657
    for(value_type i{} ; i != _length ; ++i) {
658
    if (i!=0) std::cout << " ";</pre>
```

```
else std::cout << '{';
    for (value_type j{}; j != _length; ++j) {
    std::cout << "(" << _v_bonds[i][j].get_groupID() << ":" << _v_bonds[i
     ][i] << ")";</pre>
    if(j != _length -1)
663
    std::cout << ',';
664
665
    std::cout << '}';
666
    if(i != _length -1)
    std::cout << std::endl;</pre>
    std::cout << '}';
    std::cout << std::endl;</pre>
671
672
673
674
    /**
675
676
    */
    void SqLattice::view_bonds_by_id(){
    std::cout << "Bonds by id: line" << __LINE__ << endl;
    cout << "Structure " << endl;</pre>
680
    print_h_barrier(8, "__", "___", "_\n");
681
                   (horizontal bond id)|" << endl;</pre>
    cout << "
682
    cout << "|( vertical bond id)</pre>
                                   |" << end1;
683
    print_h_barrier(8, "---", "-\n");
684
    // printing indices for columns
    std::cout << " | ";
    for(value_type i{}; i != _length; ++i){
    std::cout << i << " | ";
689
    std::cout << std::endl;</pre>
690
691
    // pringing H,V label
692
    694
    print_h_barrier(_length , "____|_", "____|_");
    // for each row there will be two columns
    for(value_type i{}; i != _length; ++i){
698
    std::cout << i << ' ';
699
    std::cout << "H |";
700
    for(value_type j1{}; j1 != _length; ++j1){
```

```
std::cout << " " << std::setw(3) << _h_bonds[i][j1].get_groupID() <<
       "|";
703
     std::cout << std::endl;
704
     std::cout << " " << "V | ";
705
     for(value_type j2{}; j2 != _length; ++j2){
706
     std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "
707
708
     std::cout << std::endl;</pre>
709
     // printing horizontal separator
711
     print_h_barrier(_length , "____|_", "____|_");
712
     }
713
714
     11
                view_h_bonds_extended();
     11
                view_v_bonds_extended();
716
     std::cout << std::endl;
718
     }
     Site& SqLattice::getSite(Index index) {
     return _sites[index.row_][index.column_];
     }
723
724
     // Site&& SqLattice :: getSiteR (Index index) {
725
     //
           Site a = \_sites[index.x_][index.y_];
726
     //
           return std::move(a);
727
     //}
728
729
     const Site& SqLattice::getSite(Index index) const {
730
     return _sites[index.row_][index.column_];
731
     }
732
     void SqLattice::setGroupID(Index index, int group_id){
734
     _sites[index.row_][index.column_].set_groupID(group_id);
735
736
     void SqLattice::setGroupID(BondIndex index, int group_id){
738
     if (index . horizontal()){
739
     _h_bonds[index.row_][index.column_].set_groupID(group_id);
740
741
     if (index.vertical()){
742
     _v_bonds[index.row_][index.column_].set_groupID(group_id);
743
744
```

```
745
     int SqLattice::getGroupID(Index index){
     return _sites[index.row_][index.column_].get_groupID();
748
749
750
     int SqLattice::getGroupID(BondIndex index){
751
     if (index.horizontal()){
752
     return _h_bonds[index.row_][index.column_].get_groupID();
753
     if (index.vertical()){
755
     return _v_bonds[index.row_][index.column_].get_groupID();
756
757
     return -1;
758
759
760
     //Bond Lattice::get_h_bond(Index set_ID) {
761
     //
           return _h_bonds[id.x_][set_ID.y_];
762
     //}
763
     //
     //Bond Lattice::get_v_bond(Index set_ID) {
765
           return _v_bonds[id.x_][set_ID.y_];
766
     //}
767
768
769
    Bond& SqLattice::get_h_bond(Index id) {
770
     return _h_bonds[id.row_][id.column_];
771
772
773
    Bond& SqLattice::get_v_bond(Index id) {
774
     return _v_bonds[id.row_][id.column_];
775
     }
776
777
778
     Bond& SqLattice::getBond(BondIndex index) {
779
     if (index.horizontal())
780
     return _h_bonds[index.row_][index.column_];
     if (index.vertical())
     return _v_bonds[index.row_][index.column_];
783
     // todo throw exception
784
     throw InvalidBond {"Invalid bond : line " + to_string(__LINE__) };
785
786
787
     void SqLattice::reset(bool reset_all) {
788
```

```
if (reset_all){
789
     reset_sites();
     reset_bonds();
791
     return;
792
793
     // setting all group id to -1
794
     if(_site_resetting_flag) {
795
     reset_sites();
796
     }
797
     //
           cout << "Bond resetting is disabled : line " << __LINE__ << endl
     if(_bond_resetting_flag) {
     reset_bonds();
800
801
802
803
     }
804
     /**
805
     */
807
     void SqLattice::reset_bonds() {
808
     for(value_type i{}; i != _h_bonds.size(); ++i){
809
     for (int j{}; j != _h_bonds[i].size(); ++j) {
810
     // deactivating. automatically set group id == - and relative index ==
811
       (0,0)
     // setting group id = -1 and deactivating the bond
812
     _h_bonds[i][j].deactivate();
813
     _v_bonds[i][j].deactivate();
815
816
     }
817
818
     }
819
820
     /**
821
822
     */
823
     void SqLattice::reset_sites() {
     for(value_type i{}; i != _sites.size(); ++i){
825
     for(value_type j{}; j != _sites[i].size(); ++j) {
826
     // deactivating. automatically set group id == - and relative index ==
827
       (0,0)
     // setting group id = -1 and deactivating the site
828
     _sites[i][j].deactivate();
```

```
833
834
835
836
    * Get Neighbor from given index
837
838
      ************************
      */
839
    * Periodic case only.
840
    * Each site has four neighbor sites.
841
    * @param site
    * @return
843
844
    */
    std::vector < Index > SqLattice::get_neighbor_site_indices (Index site) {
    std::vector<Index> sites(4);
    sites[0] = \{(site.row_+ 1) \% _length, site.column_\};
847
    sites[1] = {(site.row_ - 1 + _length) \% _length, site.column_};
848
    sites[2] = { site.row_, (site.column_ + 1) % _length };
849
    sites[3] = {site.row_, (site.column_ - 1 + _length) \% _length};
850
    return sites;
851
852
    }
    /**
    * Periodic case only.
    * Each bond has six neibhbor bonds.
856
    * @param site
857
    * @return
858
    */
859
    std::vector <BondIndex > SqLattice::get_neighbor_bond_indices(BondIndex
860
    value_type next_column = (bond.column_ + 1) % _length;
    value_type prev_column = (bond.column_ - 1 + _length) % _length;
    value_type prev_row = (bond.row_ - 1 + _length) % _length;
863
    value_type next_row = (bond.row_ + 1) % _length;
864
865
    vector < BondIndex > bonds(6);
866
867
    // horizontal bond case
868
```

```
if (bond.horizontal()) {
     // increase column index for the right neighbor
871
     // left end of bond
872
     bonds[0] = {BondType:: Vertical, bond.row_, bond.column_};
873
     bonds[1] = {BondType:: Vertical, prev_row, bond.column_};
874
     bonds[2] = {BondType::Horizontal, bond.row_, prev_column};
875
876
     // right end bond
877
     bonds[3] = {BondType:: Vertical, prev_row, next_column};
     bonds[4] = {BondType:: Vertical, bond.row_, next_column};
879
     bonds[5] = {BondType::Horizontal, bond.row_, next_column};
881
882
     // vertical bond case
883
     else if (bond.vertical()) {
884
     // increase row index
886
     // top end of bond
     bonds[0] = {BondType::Horizontal, bond.row_, bond.column_};
     bonds[1] = {BondType::Horizontal, bond.row_, prev_column};
889
     bonds[2] = {BondType:: Vertical, prev_row, bond.column_};
890
891
     // bottom end of bond
892
     bonds[3] = {BondType::Horizontal, next_row, bond.column_};
893
     bonds[4] = {BondType:: Horizontal, next_row, prev_column};
894
     bonds[5] = {BondType:: Vertical, next_row, bond.column_};
895
     }
897
899
     return bonds;
900
901
902
     std::vector<Index> SqLattice::get_neighbor_indices(BondIndex bond) {
903
     value_type r = bond.row_;
904
     value_type c = bond.column_;
     vector < Index > sites(2);
     sites[0] = \{r, c\};
907
     if (bond.horizontal()){
908
     sites [1] = \{r, (c+1) \% \_length\};
909
     } else {
910
     sites [1] = \{(r+1) \% \text{ length}, c\};
911
912
```

```
return sites;
916
    * Static methods
917
     */
918
    std::vector < Index > SqLattice::get_neighbor_site_indices(size_t length,
919
       Index site){
     std::vector<Index> sites(4);
920
     sites[0] = {(site.row_ + 1) \% length, site.column_};
     sites [1] = \{ (site.row_ - 1 + length) \% length, site.column_ \};
     sites[2] = { site.row_, (site.column_ + 1) % length };
     sites[3] = \{ site.row\_, (site.column\_ - 1 + length) \% length \};
924
     return sites;
925
     }
926
927
    /**
928
    * Periodic case only.
929
    * Each bond has six neibhbor bonds.
    * @param site
    * @return
932
     */
933
    std::vector <BondIndex > SqLattice::get_neighbor_bond_indices(size_t
934
     length, BondIndex bond) {
    value_type next_column = (bond.column_ + 1) % length;
935
     value_type prev_column = (bond.column_ - 1 + length) % length;
936
     value_type prev_row = (bond.row_ - 1 + length) % length;
937
     value_type next_row = (bond.row_ + 1) % length;
     vector < BondIndex > bonds(6);
941
     // horizontal bond case
942
     if (bond.horizontal()) {
943
     // increase column index for the right neighbor
944
     // left end of bond
     bonds[0] = {BondType:: Vertical, bond.row_, bond.column_};
     bonds[1] = {BondType:: Vertical, prev_row, bond.column_};
     bonds[2] = {BondType::Horizontal, bond.row_, prev_column};
950
     // right end bond
951
     bonds[3] = {BondType:: Vertical, prev_row, next_column};
952
     bonds[4] = {BondType:: Vertical, bond.row_, next_column};
953
     bonds[5] = {BondType::Horizontal, bond.row_, next_column};
954
```

```
955
     // vertical bond case
     else if (bond.vertical()) {
958
     // increase row index
959
960
     // top end of bond
961
     bonds[0] = {BondType:: Horizontal, bond.row_, bond.column_};
962
     bonds[1] = {BondType::Horizontal, bond.row_, prev_column};
963
     bonds[2] = {BondType:: Vertical, prev_row, bond.column_};
     // bottom end of bond
     bonds[3] = {BondType::Horizontal, next_row, bond.column_};
967
     bonds[4] = {BondType::Horizontal, next_row, prev_column};
968
     bonds[5] = {BondType:: Vertical, next_row, bond.column_};
969
970
     }
971
972
     return bonds;
975
976
     std::vector < Index > SqLattice::get_neighbor_indices(size_t length,
977
      BondIndex bond) {
     value_type r = bond.row_;
978
     value_type c = bond.column_;
979
     vector < Index > sites(2);
980
     sites[0] = \{r, c\};
     if (bond.horizontal()){
982
     sites [1] = \{r, (c+1) \% length\};
     } else {
984
     sites [1] = \{(r+1) \% \text{ length }, c\};
985
986
     return sites;
987
989
```

A.2.4 Cluster

file: cluster.h

```
//
2 // Created by shahnoor on 10/3/2017.
```

```
//
    #ifndef SITEPERCOLATION_CLUSTER_H
    #define SITEPERCOLATION CLUSTER H
    #include <vector>
    #include <set>
   #include "../lattice/bond.h"
   #include "../types.h"
    #include "../lattice/site.h"
    /**
15
    * Cluster of bonds and sites
   * version 3
17
   * final goal -> make a template cluster. so that we can use it for
    Bond cluster or Site cluster
   * root site (bond) is the first site (bond) of the cluster. nedeed for
      (wrapping) site percolation
    */
    class Cluster {
    // contains bond and site
    std::vector<BondIndex> _bond_index; // BondIndex for indexing bonds
    std:: vector < Index >
                            _site_index; // Site index
24
25
26
    int _creation_time; // holds the creation birthTime of a cluster
27
    object
    int _id;
    public:
        using iterator = std::vector < Bond >::iterator;
31
    ~Cluster()
                                          = default;
32
    Cluster()
                                          = default;
33
    Cluster (Cluster &)
                                      = default;
    Cluster (Cluster & &)
                                      = default;
35
    Cluster& operator = (const Cluster&) = default;
    Cluster& operator = (Cluster&&) = default;
    explicit Cluster(int id){
39
    _id = id; // may be modified in the program
41
42
    /*
43
```

```
* Only readable, not modifiable.
    * when time = 0 => only lattice exists and bonds in site percolation,
     not any sites
    * When id = 0, time = 1 => we have placed the first site, hence
     created a cluster with size greater than 1
           Only then Cluster constructor is called.
48
    */
49
    _creation_time = id + 1; // only readable, not modifiable
    void addSiteIndex(Index);
54
    void addBondIndex (BondIndex );
55
    Index lastAddedSite(){return _site_index.back();}
57
    BondIndex lastAddedBond() { return _bond_index . back(); }
59
    bool isPresent(BondIndex bond) const ;
    bool isPresent(Index site) const ;
    bool checkPresenceAndErase(BondIndex bond);
63
    bool checkPresenceAndErase(Index bond);
64
    bool checkPresenceAndEraseIf(BondIndex bond, bool flag);
    bool checkPresenceAndEraseIf(Index bond, bool flag);
67
    void eraseSite(value_type index);
    void eraseBond(value_type index);
72
    void insert(const std::vector < BondIndex > & bonds);
73
    void insert(const std::vector<Index>& sites);
74
    void insert(const Cluster& cluster);
    void insert_v2(const Cluster& cluster);
    void insert_with_id_v2(const Cluster& cluster, int id);
    friend std::ostream& operator <<(std::ostream& os, const Cluster&
81
     cluster);
82
    const std::vector < BondIndex > & getBondIndices()
                                                        { return
     _bond_index;}
```

```
const std::vector<Index>&
                                      getSiteIndices()
                                                           { return
      _site_index;}
    const std::vector < BondIndex > &
                                      getBondIndices()
                                                        const {return
      bond index;}
    const std::vector<Index>&
                                      getSiteIndices()
                                                        const {return
      _site_index;}
    value_type numberOfBonds() const { return _bond_index.size();}
89
    value_type numberOfSites() const { return _site_index.size();}
    int get_ID() const { return _id;}
    void set_ID(int id) { _id = id;}
93
    int birthTime() const {return _creation_time;}
94
95
    Index getRootSite()const{return _site_index[0];} // for site
96
      percolation
    BondIndex getRootBond()const{return _bond_index[0];} // for bond
97
      percolation
    bool empty() const { return _bond_index.empty() && _site_index.empty()
    void clear() {_bond_index.clear(); _site_index.clear(); }
99
    };
100
101
102
103
    #endif //SITEPERCOLATION CLUSTER H
104
106
```

file: cluster.cpp

```
// Created by shahnoor on 10/2/2017.

//

// Created by shahnoor on 10/11/2017.

//

// Created by shahnoor on 10/11/2017.

//

using namespace std;
```

```
14
    // add Site index
    void Cluster::addSiteIndex(Index index) {
    _site_index.push_back(index);
17
18
19
    void Cluster::addBondIndex(BondIndex bondIndex) {
20
    _bond_index.push_back(bondIndex);
21
    }
22
24
    bool Cluster::isPresent(BondIndex bond) const {
    for (auto a: _bond_index) {
26
    if (a == bond)
27
    return true;
28
29
    return false;
30
31
    bool Cluster::isPresent(Index site) const {
    for (auto a: _site_index) {
34
    if (a == site)
35
    return true;
36
    return false;
38
39
    bool Cluster::checkPresenceAndErase(BondIndex bond) {
    for (auto it = _bond_index.begin(); it != _bond_index.end(); ++it) {
42
    if (* it == bond) {
43
    _bond_index . erase(it);
44
    return true;
45
46
47
    return false;
49
    bool Cluster::checkPresenceAndEraseIf(BondIndex bond, bool flag) {
51
    if (! flag)
    return false;
53
    for (auto it = _bond_index.begin(); it != _bond_index.end(); ++it) {
    if (* it == bond) {
    _bond_index.erase(it);
    return true;
```

```
return false;
60
61
62
     bool Cluster::checkPresenceAndEraseIf(Index bond, bool flag) {
63
    if (!flag)
64
    return false;
65
    for (auto it = _site_index.begin(); it != _site_index.end(); ++it) {
    if (* it == bond) {
     _site_index.erase(it);
     return true;
    }
70
71
    return false;
72
73
74
75
    bool Cluster::checkPresenceAndErase(Index bond) {
76
     for (auto it = _site_index.begin(); it != _site_index.end(); ++it) {
     if (* it == bond) {
78
     _site_index.erase(it);
79
     return true;
80
81
82
    return false;
83
84
    }
    void Cluster::eraseSite(value_type index) {
87
     auto it = _site_index.begin();
     it += index;
     _site_index.erase(it);
90
91
    void Cluster::eraseBond(value_type index) {
93
    auto it = _bond_index.begin();
     it += index;
     _bond_index.erase(it);
    }
97
98
99
    void Cluster::insert(const std::vector < BondIndex > & bonds) {
100
    _bond_index.reserve(bonds.size());
101
```

```
for(value_type i{} ; i != bonds.size() ; ++i){
    _bond_index.push_back(bonds[i]);
104
105
    }
106
    void Cluster::insert(const std::vector<Index>& sites){
107
    _site_index.reserve(sites.size());
108
    for(value_type i{} ; i != sites.size() ; ++i){
109
    _site_index.push_back(sites[i]);
110
    }
113
114
    * Merge two cluster as one
115
    * All intrinsic property should be considered, e.g., creation time of
116
      a cluster must be recalculated
    * @param cluster
118
    */
    void Cluster::insert(const Cluster &cluster) {
    if (_id > cluster._id){
    cout << "_id > cluster._id : line " << __LINE__ << endl;</pre>
    _id = cluster._id;
    // older time or smaller time is the creation birthTime of the cluster
124
           cout << "Comparing " << _creation_time << " and " << cluster.</pre>
125
      _creation_time;
    _creation_time = _creation_time < cluster._creation_time ?
126
      _creation_time : cluster._creation_time;
           cout << " Keeping " << _creation_time << endl;</pre>
127
    _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
128
      cluster._bond_index.end());
    _site_index.insert(_site_index.end(), cluster._site_index.begin(),
129
      cluster._site_index.end());
130
    }
132
    /**
    * Merge two cluster as one
134
    * All intrinsic property should be considered, e.g., creation time of
135
      a cluster must be recalculated
    * @param cluster
136
    */
    void Cluster::insert_v2(const Cluster &cluster) {
138
    // older time or smaller time is the creation birthTime of the cluster
```

```
cout << "Comparing " << _creation_time << " and " << cluster.
      _creation_time;
141
     _creation_time = _creation_time < cluster._creation_time ?
      creation time: cluster. creation time;
           cout << " Keeping " << _creation_time << endl;</pre>
142
     _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
143
      cluster._bond_index.end());
     _site_index . insert(_site_index . end(), cluster . _site_index . begin(),
144
      cluster._site_index.end());
     void Cluster::insert_with_id_v2(const Cluster &cluster, int id) {
148
     _id = id;
149
    // older time or smaller time is the creation birthTime of the cluster
150
           cout << "Comparing " << _creation_time << " and " << cluster.</pre>
      _creation_time;
     _creation_time = _creation_time < cluster._creation_time ?
      _creation_time : cluster._creation_time;
           cout << " Keeping " << _creation_time << endl;</pre>
     //
153
     _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
154
      cluster._bond_index.end());
     _site_index . insert(_site_index . end(), cluster . _site_index . begin(),
      cluster._site_index.end());
156
157
158
     std::ostream &operator <<(std::ostream &os, const Cluster &cluster) {
    os << "Sites : size (" << cluster._site_index.size() << ") : ";
160
    os << '{';
161
     for(auto a: cluster._site_index){
162
    os << a << ',';
163
164
    os << '}' << endl;
165
    os << "Bonds : size (" << cluster._bond_index.size() <<") : ";
167
     os << '{';
     for(auto a: cluster._bond_index){
    os << a << ',';
170
     }
    os << '}';
173
     return os << endl;</pre>
174
175
```

```
176
177
```

A.2.5 Percolation

file: cluster.h

```
\begin{array}{ccc}
a & = & -1 \\
2 & & & & \\
\end{array}
```

A.2.6 Utility

A.2.7 Tests

A.2.8 Main

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

B.1 Algorithm

One further slightly tricky point in the implementation of our scheme is the performance of the convolution, Eq. (2), of the results of the algorithm with the binomial distribution. Since the number of sites or bonds on the lattice can easily be a million or more, direct evaluation of the binomial coefficients using factorials is not possible. And for high-precision studies, such as the calculations presented in Section III, a Gaussian approximation to the binomial is not sufficiently accurate. 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. (We will fix it in a moment.) 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. **site to Ziff paper**

B.2 Code

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

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 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 $y' = y * L^{-ex}$

(c) get the maximum value or the peak value of y' as $y'_{max} = max(y')$ for each length

- (d) if the y'_{max} values for different exponents does not lie in the order of 10 then scale $y'_{max} = y'_{max}/max(y'_{max})$ to normalize y'_{max} . By order of 10 I mean that if the order y'_{max} for ex_i is 10^-1 and for ex_j is 10^-2 then when comparing between std_{ex_i} and std_{ex_j} we will get the std_{ex_j} is lower always. Thus just because the standard deviation is lower we cannot say it is the best exponent if the order of y'_{max} is different.
- (e) find the standard deviation of all the y'_{max} 's and call it std_{ex} 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 ex^* . Symbolically

$$ex^* = argmin_{ex \in E} \ std_{ex} \tag{C.1}$$

exponent for scaling the x-values

Usually the exponent that scales the x-values is called 1/v. 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 $\log(L)$ where || denotes the absolute value.
- 4. slope of this graph is the estimate for the exponent 1/v

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 $(1/nu)_a pprox$ 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

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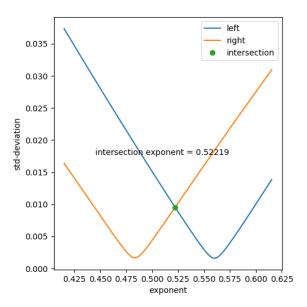


Fig. C.1 Best collapsing on either right or left ??

- 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 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 ??. 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

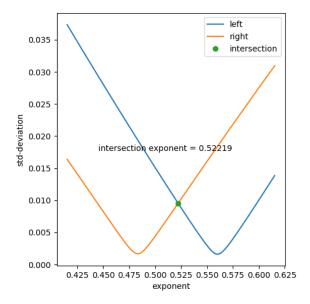


Fig. C.2 Minimizing exponent for scaling *x*-values

- 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.2 gives the visual of the above process.