Long range Interaction in Site Percolation

on Square Lattice

Muhammad Shahnoor Rahman

Department of Physics
University of Dhaka

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

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and 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
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Acknowledgements

And I would like to acknowledge ...

Abstract

This is where you write your abstract ...

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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 $[\rho] = FL^{-4}T^{-2}$ **??**[dim].

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, ... etc. When investigating a certain dimensional physical quantity (governed) that depend on other n dimensional variables then this theorem provide us a systematic way to reduce the degrees of freedom of a function. Using this theorem we reduce a function of n variables problems into a function of k dimensionless variable problem if each of the k dimensional variable of original n variables can be expressed in terms of the $n-k$ dimensionally independent variable.

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

$$a = f(a_1, a_2, \ldots, a_3) \tag{2.1}$$

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

$$[a_1] = [a_{k+1}]^{\alpha_1} \ldots [a_n]^{\gamma_1}$$
$$[a_2] = [a_{k+1}]^{\alpha_2} \ldots [a_n]^{\gamma_2} \tag{2.2}$$
$$\vdots \tag{2.3}$$
$$[a_k] = [a_{k+1}]^{\alpha_k} \ldots [a_n]^{\gamma_k}$$

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

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

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

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

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

$$\vdots \tag{2.7}$$

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

and a dimensionless governed parameter

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

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

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

The quantities $\Pi, \Pi_1, \dots, \Pi_k$ 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 $a_{k+1}, \dots, a_n$, say for example, a_{k+1}, is changed by an arbitrary factor, and the remaining ones are unchanged. Upon such transition the first argument of F is unchanged arbitrarily, and all other arguments of the function remain unchanged as well as its value Π. Hence, it follows $\frac{\delta F}{\delta a_{k+1}} = 0$ and entirely analogously $\frac{\delta F}{\delta a_{k+2}} = 0, \dots, \frac{\delta F}{\delta a_n} = 0$. Therefore, the relation 2.10 is in fact represented by a function of k arguments and proves it is independent of $a_{k+1}, \dots, a_n$, that is,

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

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

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

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

$$[a] \sim [c] \text{ and } [b] \sim [c] \tag{2.14}$$

and so is true for the governed parameter S as we can write the dimensional relation $[S] \sim \left[c^2\right]$. 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

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

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 param- eters, i.e. the lengths of the sides, while the dimensionless parameters, the angles at the vertices are identical for the two triangles. Analogously,
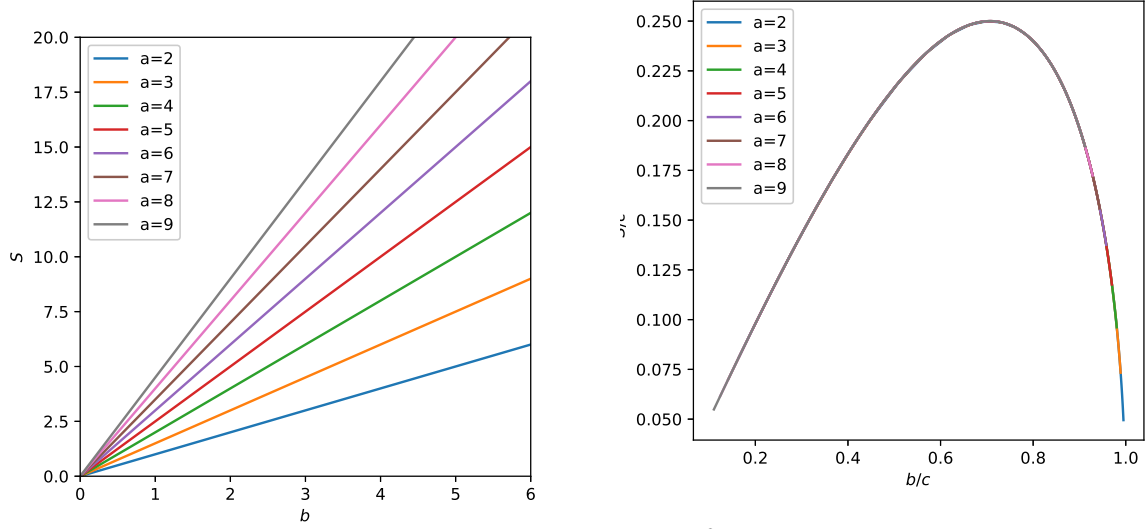
(a) *S* vs *b* graph. *b* is the base of the triangle which is varied for a single θ.

(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 $\Pi_1, \ldots, \Pi_k$ 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

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

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

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

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

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

and

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

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
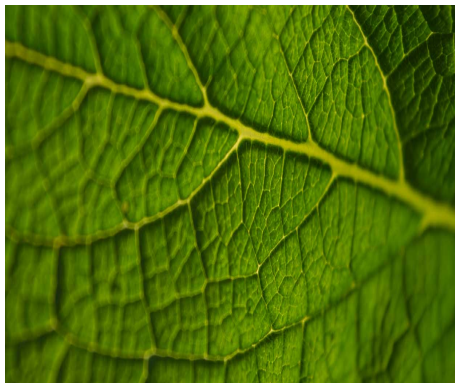
(a) Leaf

(b) Snowflake

(c) Blood vessel

(d) Leafless Tree

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 $\left[t^\theta\right] = [f]$ 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

$$x \rightarrow \lambda^z x \tag{2.36}$$
$$t \rightarrow \lambda t \tag{2.37}$$
$$f \rightarrow \lambda^\theta \tag{2.38}$$

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

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

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

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

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

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

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

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

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 ν via $\theta = -\omega/\nu$.

A quantitative way of interpreting how the experimental data exhibits finite-size scaling is done by invoking the idea of data-collapse method - an idea that goes back to the original

observation of Rushbrooke. That is, the values of $f(\varepsilon, L)$ for different system size L can be made to collapse on a single curve if $fL^{\omega/\nu}$ is plotted against $\varepsilon L^{1/\nu}$. It implies that systems of different sizes are all similar that also include system where $L \to \infty$. 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

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

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

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

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

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

This is a first order differential equation which has a solution

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

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

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

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,

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

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

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

$$dE = dQ - PdV \tag{3.2}$$

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

$$dQ = TdS?? \tag{3.3}$$

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

$$dE = TdS - pdV \tag{3.4}$$

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

$$dE = TdS - pdV$$
$$= TdS + SdT - SdT - PdV$$
$$d(E - TS) = -SdT - PdV$$
$$dA = -SdT - PdV \tag{3.6}$$

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

$$dA = -SdT - PdV - VdP + VdP$$
$$d(A + PV) = -SdT + VdP$$
$$dG = -SdT + VdP \tag{3.7}$$

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 Definition of Thermodynamic Quantities

3.2.1 Entropy

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.

Entropy in one of the key feature of a phase transition model. But thermodynamic entropy cannot be calculated for any model such as our percolation on a square lattice model. So we take our approach in another way. Information entropy or the Shanon entropy is best suited for our model. The concept of information entropy was introduced by Claude Shannon in his 1948 paper "A Mathematical Theory of Communication" [22]. The Defition is

$$H = -\sum_i \mu_i \log \mu_i \qquad (3.8)$$

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

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

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

so in this system entropy is 1.

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

(a) Free particles. $H = 3$

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

(c) Bount particles. $H = 0$
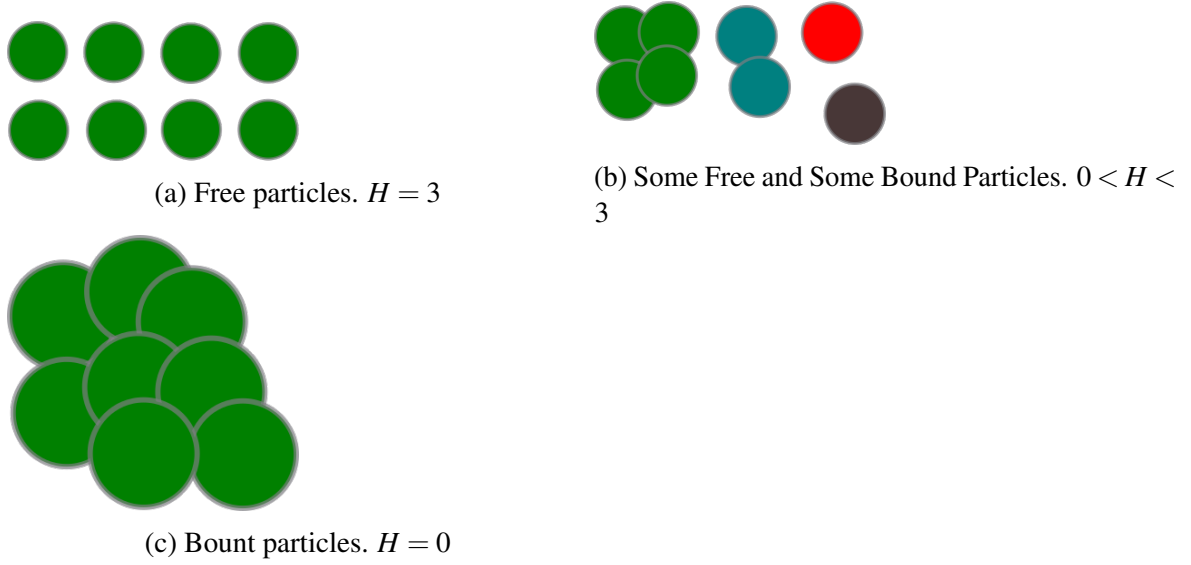
Fig. 3.1 entropy of a system of 8 particles

entropy of the system becomes,

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

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.

The reason I am taking the system size as 2^n for all n is that it's easier to take logarithm of base 2.

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

3.2.4 Order Parameter

3.2.5 Susceptibility

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

$$dE = TdS - PdV \tag{3.9}$$

for a magnetic system $P \rightarrow h$ and $V \rightarrow -m$, where h is the magnetic field and m is the magnetization. The negative sign for the magnetization is because of the fact that the magnetization increases with the increase of the magnetic field whereas the volume decreases as the pressure increases. Since we relate pressure to the magnetic field, to relate volume to magnetization we need to put a minus sign with it. Thus we get

$$dE = TdS + hdm \tag{3.10}$$
$$= TdS + SdT - SdT + hdm \tag{3.11}$$
$$d(E - TS) = -SdT + hdm \tag{3.12}$$
$$dA = -SdT + hdm \tag{3.13}$$
$$dA = -SdT + hdm + mdh - mdh \tag{3.14}$$
$$d(A - mh) = -SdT - mdh \tag{3.15}$$
$$dG = -SdT - mdh \tag{3.16}$$

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 3.16 3.13 we can find the expression for entropy and magnetization in terms of free energy.

$$S = -\left(\frac{\partial G}{\partial T}\right)_h = -\left(\frac{\partial A}{\partial T}\right)_m \tag{3.17}$$

$$m = -\left(\frac{\partial G}{\partial h}\right)_T \tag{3.18}$$

$$h = \left(\frac{\partial A}{\partial m}\right)_T \tag{3.19}$$

(a) negative slope   (b) positive slope
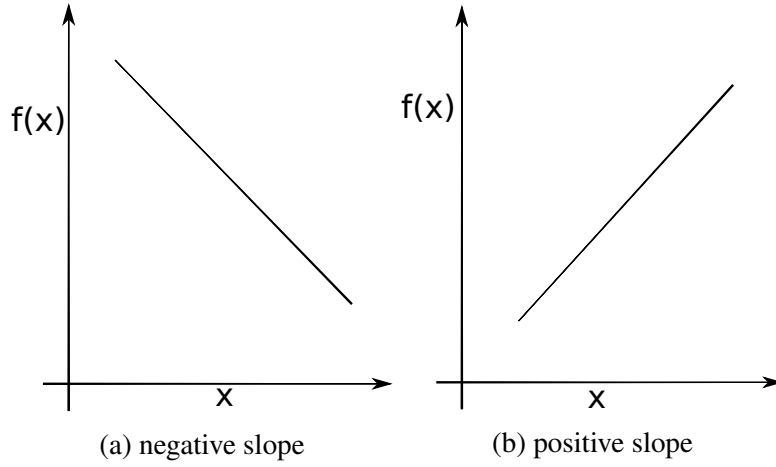
Fig. 3.2 shape of $f(x)$ from $f'(x)$

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

$$\chi = \left(\frac{\partial m}{\partial h}\right)_h = -\left(\frac{\partial^2 G}{\partial h^2}\right)_T \tag{3.20}$$

again we can write χ as

$$\chi = \frac{1}{\frac{\partial h}{\partial m}}$$
$$= \frac{1}{\frac{\partial^2 A}{\partial m^2}} \tag{3.21}$$

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.

(a) concave   (b) convex
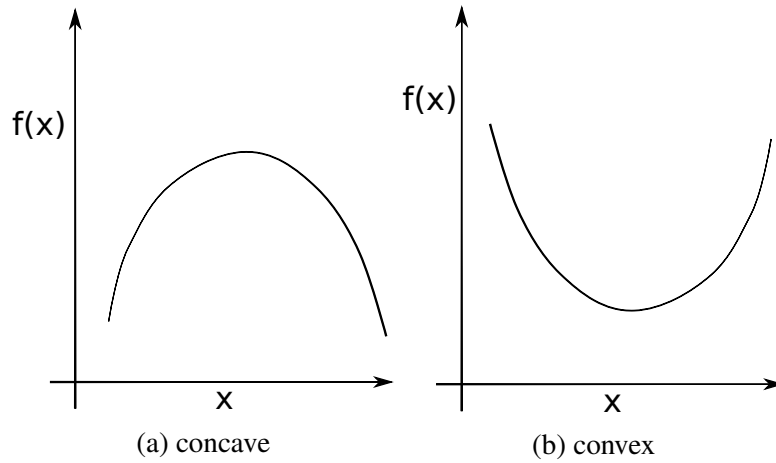
Fig. 3.3 shape of $f(x)$ from $f''(x)$
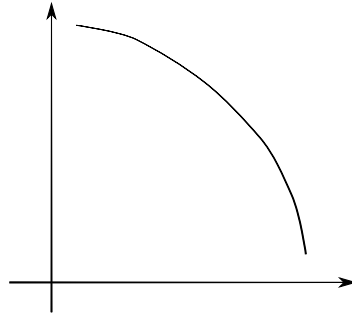
Fig. 3.4 Shape of the free energy

3.3.2   Free Energy

Now since we obtain from 3.7 that the entropy is the first derivative of the free energy 3.22 and from 3.27 specific heat is the second derivative of the free energy 3.23. 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 that the shape of the free energy should be a decreasing concave curve 3.4 in other words concave shaped with negative slope.

$$S = -\frac{\partial G}{\partial T} \tag{3.22}$$

$$C = -\frac{\partial^2 G}{\partial T^2} \tag{3.23}$$

(a) Entropy in first order transition

(b) Entropy in 2nd order transition
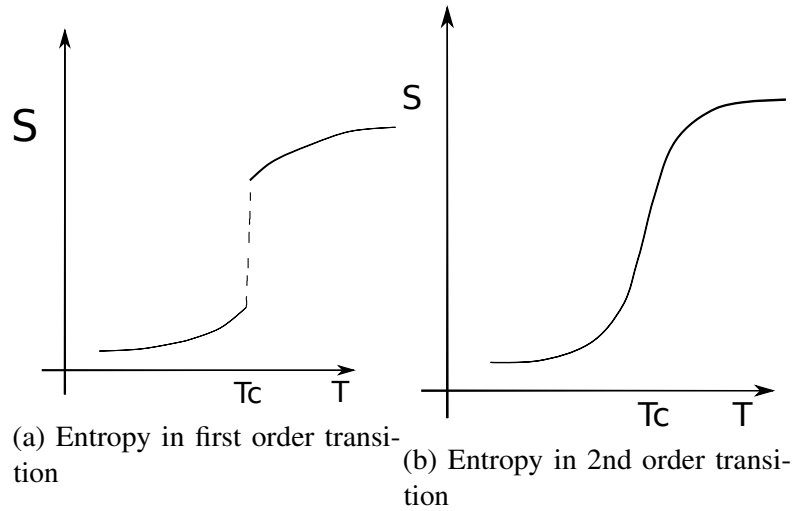
Fig. 3.5 Shape of entropy

3.3.3 Entropy and Specific Heat

Now that we know the shapes of the free energy, the very next thing to do is to find the shape of the entropy. Since we can get entropy from differentiating the free energy with respect to temperature T we get the following shape 3.5. From the definition of the transition order we know that the first order transition is discontinuous and the second order transition continuous. Since the first order transition requires latent heat at the critical point the discontinuity is inevitable. Note that, since entropy measures disorderedness of a system it should increase with increasing temperature. Because the temperature is nothing but the average kinetic energy of the particles in the system. As the kinetic energy of the system increases with 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 3.25. 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
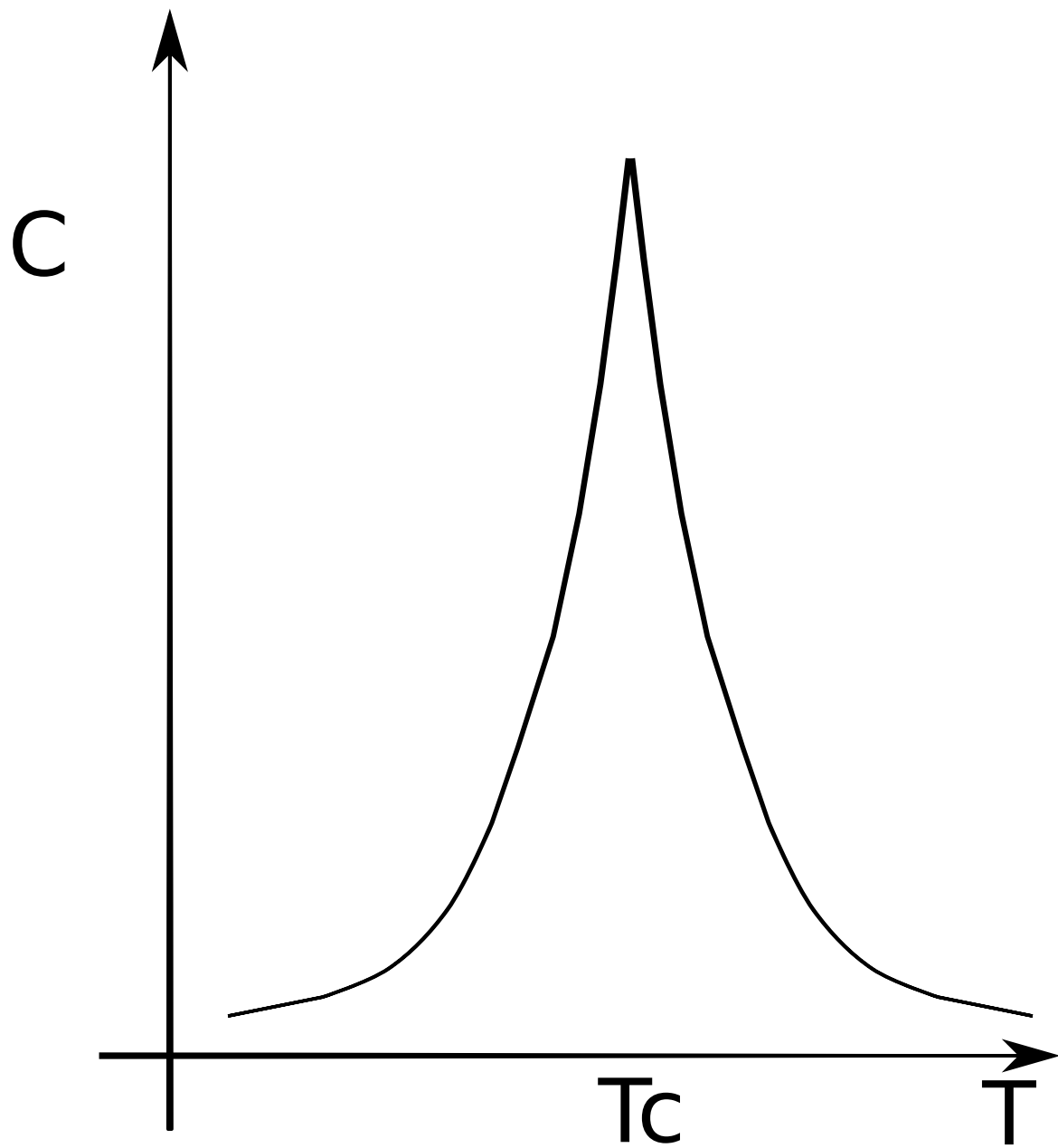
Fig. 3.6 Shape of Specific Heat

to be positive is appropriate for our model. Now if susceptibility is positive then from 3.20 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 3.18 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 3.21 we can say $\frac{\partial^2 A}{\partial m^2}$ is positive giving convex shape of the Helmholtz free energy. And 3.19 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.

$$C_x = \left(\frac{dQ}{dT}\right)_x \tag{3.24}$$

here x can be P for pressure or V for volume. And from **??** we can write

$$C_x = T\left(\frac{dS}{dT}\right) \tag{3.25}$$

To give the following

$$C_v = -T\left(\frac{\partial^2 A}{\partial T^2}\right)_v \tag{3.26}$$

$$C_p = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_p \tag{3.27}$$

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
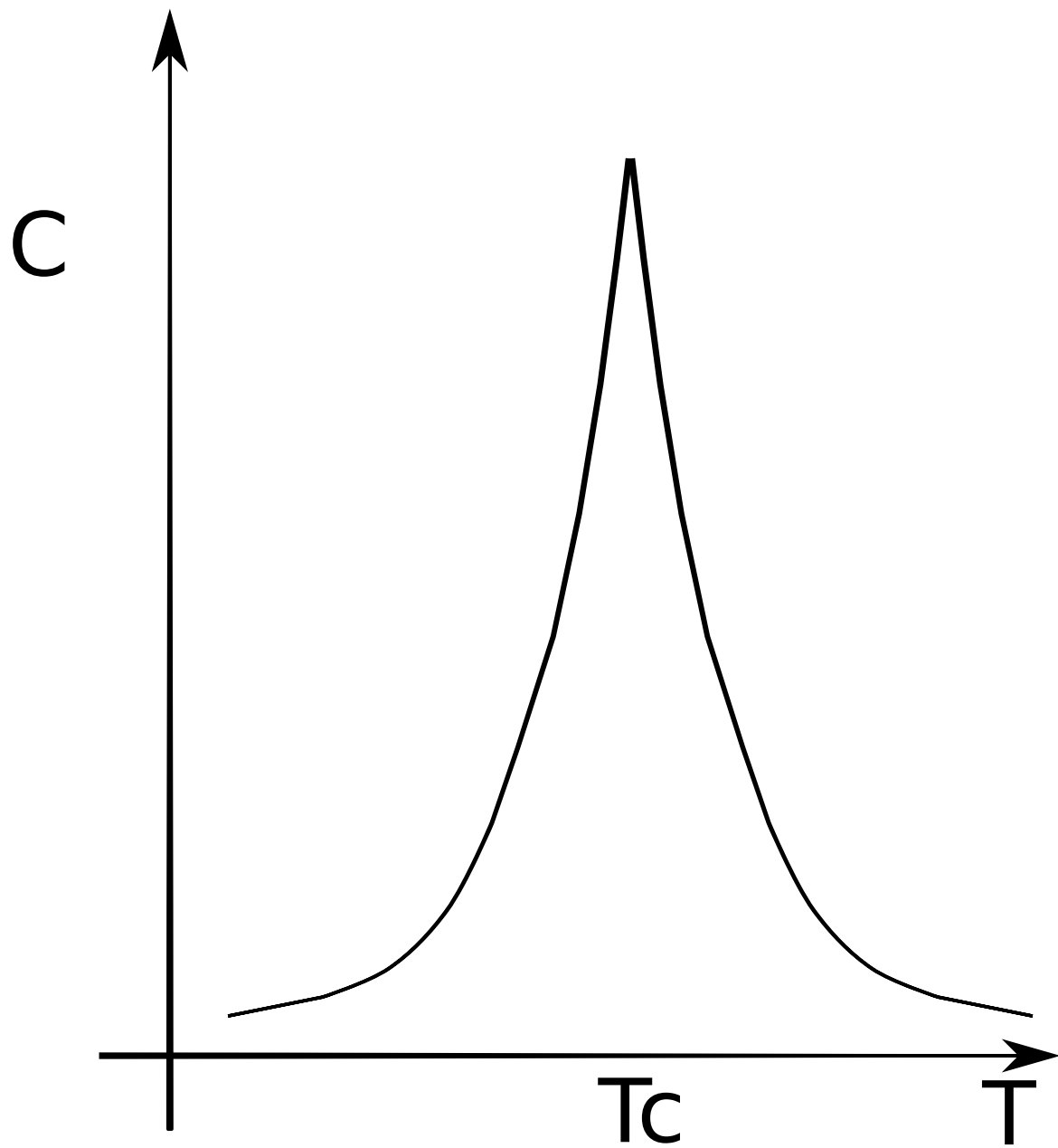
Fig. 3.7 figure required
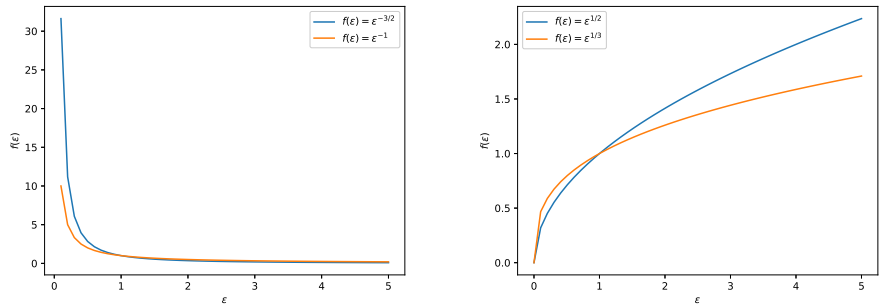
(a) $f(\varepsilon) \sim \varepsilon^{\lambda}$ where $\lambda = -1, -3/2$ (b) $f(\varepsilon) \sim \varepsilon^{\lambda}$ where $\lambda = 1/2, 1/3$

Fig. 3.8 Function showing power law

information at the critical point, $(T - T_c)/T_c$, instead of T is a better parameter to address. In equation

$$\varepsilon = \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1 \tag{3.28}$$

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 **??**

$$f(\varepsilon) \sim \varepsilon^{\lambda} \tag{3.29}$$

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

$$f(\varepsilon) = A\varepsilon^{\lambda}(1 + B\varepsilon^a + C\varepsilon^b + ...) \tag{3.30}$$

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

$$G = G(T, h) \equiv G(\varepsilon, h) \tag{3.31}$$

since ε is a better parameter. Assume that G is a generalized Homogeneous function. Therefore from **??** we can write

$$G(\lambda^{a_{\varepsilon}}\varepsilon, \lambda^{a_h}h) = \lambda G(\varepsilon, h) \tag{3.32}$$

differentiating equation 3.32 with respect to h

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

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

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

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

$$m(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) = \lambda^{1-a_h} m(\varepsilon, h) \tag{3.33}$$

$$\tag{3.34}$$

Here m is the magnetization or order parameter.

Figure of order general parameter

Setting $h = 0$ in equation 3.34

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

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

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

$$m(\varepsilon) = \varepsilon^{\beta} m(1) \tag{3.35}$$

where

$$\beta = \frac{1-a_h}{a_\varepsilon} \tag{3.36}$$

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

Setting $\varepsilon = 0$ in equation 3.34

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

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

$$m(h) = m(1)h^{\delta} \tag{3.37}$$

where

$$\delta = \frac{a_h}{1-a_h} \tag{3.38}$$

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 3.32 twice with respect to ε we get the Specific Heat

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

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

$$\lambda^{2a_\varepsilon} C(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) = \lambda C(\varepsilon, h) \tag{3.39}$$

We have used $\varepsilon = \frac{T}{T_c} - 1$ and $d\varepsilon = \frac{1}{T_c}dT$. Now setting $h = 0$ we get from 3.39

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

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

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

$$C(\varepsilon) = \varepsilon^{-\alpha} C(1) \tag{3.40}$$

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

$$\alpha = \frac{2a_\varepsilon - 1}{a_\varepsilon} \tag{3.41}$$

Again by differentiating 3.32 twice with respect to h we get the susceptibility. Then we set $h = 0$ to get only ε dependency.

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

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

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

$$\chi(\varepsilon) = \varepsilon^{-\gamma} \chi(1) \tag{3.42}$$

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

$$\gamma = \frac{2a_h - 1}{a_\varepsilon} \tag{3.43}$$

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

$$C \sim \varepsilon^{-\alpha} \tag{3.44}$$

The exponent that scales order-parameter is called β

$$m \sim \varepsilon^{\beta} \tag{3.45}$$

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

$$m \sim h^{\delta} \tag{3.46}$$

The exponent that scales susceptibility is called γ

$$\chi \sim \varepsilon^{-\gamma} \tag{3.47}$$

Note that these quantities only follows power law near T_c.

3.5.2   Rushbrooke Inequality

$$\alpha + 2\beta + \gamma \geq 2 \tag{3.48}$$

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

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

Thus the Rushbrooke inequality is satisfied.

3.5.3   Griffiths Inequality

$$\alpha + \beta(1 + \delta) = 2 \tag{3.49}$$

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

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

$$(3.50)$$

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

3.6.3   Bragg William Model

Chapter 4

Percolation Theory

4.1   Percolation Phenomena

4.2   Historical Overview

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

Bond Percolation

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

Site Percolation

In site (or vertex, node) percolation we occupy the sites. According to the definition of site percolation we use sites to measure the cluster size. But in order to keep it consistent with

the laws of thermodynamics we have changed the definition [20]. 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 [2]. 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 [21]. Determining K-cores computationally is fast and they are insightful in many situations [9, 8]. 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 [19].

Bootstrap Percolation

Bootstrap percolation is an infection-like process in which nodes becomes infected if sufficiently many of their neighbors are infected [3]. 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 $m \geq 3$, the fraction of the lattice occupied by infinite clusters discontinuously jumps from zero at the percolation threshold. From an analysis of stable and metastable ground state of the dilute Blume-Capel model [4], it is concluded that the effects like bootstrap percolation may occur in some real magnets [7].

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 [15]. 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" [17]. Various percolation processes have also been studied in several different types of multi-layer networks (e.g. multiplex networks and interdependent networks) [5, 13]. 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* [11, 18, 6], 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* [10, 16, 23]; 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 [14].
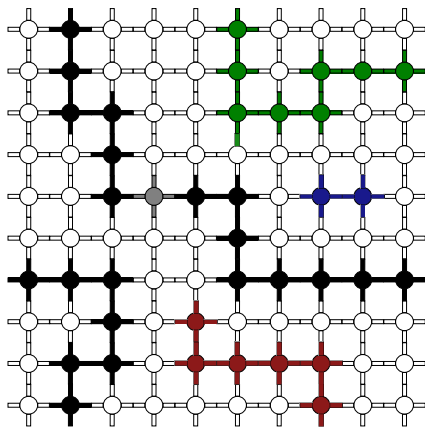
(a) One step away from threshold. Since the gray site is not occupied. The moment it gets occupied we reach percolation threshold
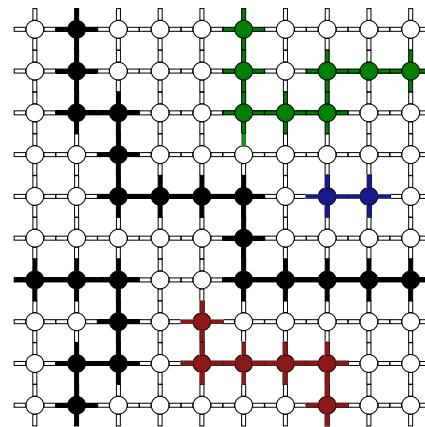
(b) The gray site gets occupied and a wrapping cluster appears for the first time. We have reached percolation threshold

Fig. 4.1 A square lattice of length $L = 10$. Demonstrating the appearance of the wrapping cluster

4.3.2 Types of Playground

Lattice

Graph

4.4 Observables

4.4.1 Percolation Threshold, p_c

4.4.2 Spanning Probability, $w(p)$

4.4.3 Entropy, $H(p,L)$

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

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

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

4.4.7 Mean Cluster Size, S

4.4.8 Cluster Size Distribution Function, n_s

$$n_s(p_c) \sim s^{-\tau} \tag{4.1}$$

4.4.9 Correlation Function, $g(r)$

4.4.10 Correlation length, ξ

4.4.11 Fractal Dimension, d_f

4.5 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.

Fig. 4.2 One Dimensional Lattice. Empty ones are white and filled ones are black.

4.5.1 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.

$$\lim_{L \to \infty} omega(p, L) = \begin{cases} 0 \, , \, \forall p < 1 \\ 1 \, \text{only if p = 1} \end{cases} \tag{4.2}$$

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

$$p_c = 1 \tag{4.3}$$

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

$$n_s = p^s(1-p)^s \tag{4.4}$$

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 4.4 gives

$$n_s = (1-p)^2 \exp(s \ln p) = (1-p)^2 \exp(-s/\xi) \tag{4.5}$$

where ξ is the correlation length and defined as

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln(p_c - (p_c - p))} \sim (p - p_c)^{-1} = (p - p_c)^{\nu} \tag{4.6}$$

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

Mean Cluster Size

The probability that an arbitrary site is in s-cluster is larger by a factor of s. This site can be any of the sites in the s-cluster. The probability that an arbitrary chosen site belongs to a cluster of size s is $n_s s$, since n_s is known to be the number of s-clusters per lattice site. Every occupied site must belong to one cluster even if it is a cluster of only one site, i.e., a cluster of size unity. The probability that an arbitrary site belongs to a cluster is therefore proportional to the probably p that it is occupied.

$$\sum_{s=1}^{\infty} s n_s = \frac{number of total occupied sites}{number of total lattice sites} = p \tag{4.7}$$

A quick check of the validity of equation 4.7 can be performed using equation 4.4.

$$
\begin{aligned}
\sum_{s=1}^{\infty} s n_s &= \sum_s s(1-p)^2 p^s \\
&= (1-p)^2 \sum_s s p^s \\
&= (1-p)^2 \sum_s p \frac{d(p^s)}{dp} \\
&= (1-p)^2 p \frac{d \sum_s p^s}{dp} \\
&= (1-p)^2 p \frac{d p(1-p)^{-1}}{dp} \\
&= (1-p)^2 p \left(\frac{1}{1-p} + \frac{p}{(1-p)^2} \right) \\
&= p \tag{4.8}
\end{aligned}
$$

Here we have used the series sum 4.9.

$$
\begin{aligned}
\sum_s p^s &= p + p^2 + p^3 + \ldots \\
&= p(1 + p + p^2 + \ldots) \\
&= p(1-p)^{-1} \tag{4.9}
\end{aligned}
$$

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

$$
w_s = \frac{n_s s}{\sum_s n_s s} \tag{4.10}
$$

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

$$
S = \sum_s w_s s \tag{4.11}
$$

This equation is very much similar to

$$
\bar{x} = \int x p(x) dx \tag{4.12}
$$

using equation 4.10 we get

$$
\begin{aligned}
S &= \frac{\sum_s n_s s^2}{\sum_s n_s s} \\
&= \sum_{s=1}^{\infty} \frac{s^2 n_s}{p} \\
&= \frac{(1-p)^2}{p} \sum_{s=1}^{\infty} s^2 p^s \\
&= \frac{(1-p)^2}{p} \left(p \frac{d}{dp} \right)^2 \left(\sum_{s=1}^{\infty} p^s \right) \\
&= \frac{(1-p)^2}{p} \left(p \frac{d}{dp} \right)^2 (p(1-p)^{-1}) \\
&= p(1-p)^2 \frac{d^2}{dp^2} (p(1-p)^{-1}) \\
&= p(1-p)^2 \frac{d}{dp} (1-p)^{-2} \\
&= p(1-p)^2 2(1-p)^{-3} \\
&= \frac{2p}{1-p} \\
&= \frac{1+p}{1-p}
\end{aligned}
\tag{4.13}
$$

we can write

$$
S(p) = \frac{1-p}{1+p} = \frac{p_c + p}{p_c - p}
\tag{4.14}
$$

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 [Hassan]

$$
S(p) \sim (p_c - p)^{-1}
\tag{4.15}
$$

We encounter the similar behaviour in the higher dimensions also.

Correlation Function and Correlation Length

The correlation function or pair connectivity $g(r)$ is the probability that a site at position r from an occupied site belongs to the same finite cluster. We are not including the contribution

of the infinite cluster. This is valid infinite cluster does not exists as long as $p < 1$. Let $r = 0$ then $g(r = 0) = 1$ since the site at $r = 0$ is the selected occupied site by definition. For 1D case a site at r to be occupied and belongs to the same finite cluster, we will need r subsequent sites and the probability of getting this is p^r. Therefore

$$g(r) = p^r \tag{4.16}$$

It can also be expressed in terms of correlation length ξ

$$g(r) = \exp(\ln(p^r)) = \exp(-r/\xi) \tag{4.17}$$

where ξ is the correlation length 4.6.

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

$$S = 1 + \sum_{r=1}^{\infty} g(r) \tag{4.18}$$

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.

4.5.2 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 4.3 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

$$A \propto V^{1-1/d} \tag{4.19}$$

now as $d \to \infty$ we have

$$A \propto V \tag{4.20}$$

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 4.3. 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

$$1 + 3 \times (1 + 2 + \ldots + 2^{r-1}) = 3.2^r - 2 \tag{4.21}$$

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

$$1 + 2 + 2^2 + 2^3 + \ldots + 2^r = 2^{r+1} - 1 \tag{4.22}$$

And if we measure the surface to volume ratio we get

$$\frac{A}{V} = \frac{number of sites in the surface}{total number of sites} = \frac{3 \times 2^{r-1}}{3 \times 2^r - 2} \tag{4.23}$$

as $r \to \infty$ we get

$$\frac{A}{V} \sim \frac{3 \times 2^{r-1}}{3 \times 2^r} = \frac{1}{2} = constant \tag{4.24}$$

Therefore Bethe lattice is indeed an infinite dimensional lattice.

Percolation Threshold

Percolation threshold of Bethe lattice is the occupation probability at which an infinite cluster appears for the first time. To find it we start walking from the origin and after one step we have $z - 1$ new bonds that is connected to $z - 1$ new sites in those direction. On the average there will be $(z - 1)p$ occupied sites. And for each site there will be another $z - 1$ branch and
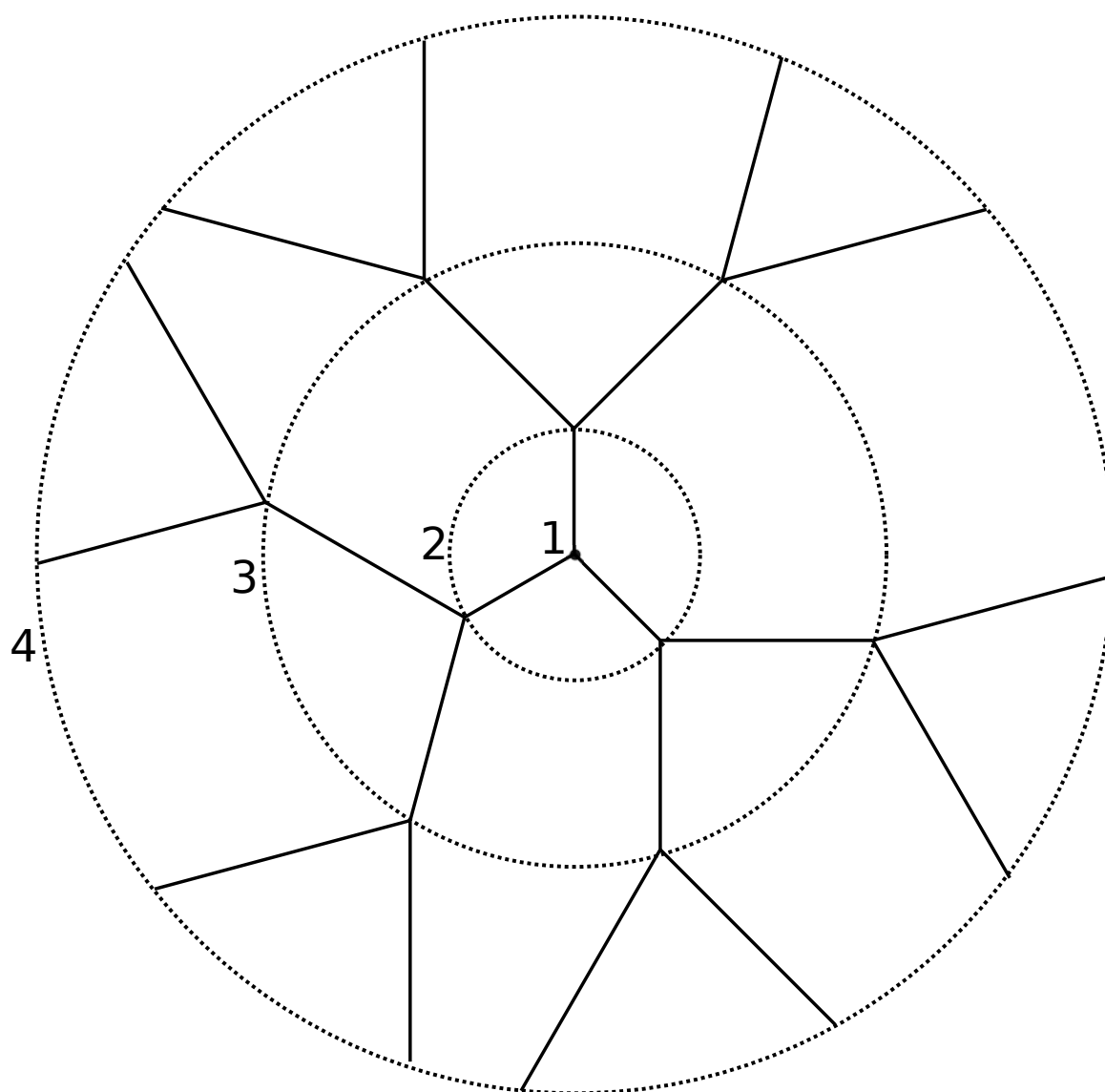
Fig. 4.3 Bethe Lattice for $z = 3$

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

$$(z-1)p_c = 1$$
$$p_c = \frac{1}{z-1} \tag{4.25}$$

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

$$P(p) = p(1 - Q^3) \tag{4.26}$$

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,

$$Q = (1-p) + pQ^2 \tag{4.27}$$

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

$$Q = 1, \frac{1-p}{p} \tag{4.28}$$

For z neighbors, in general we have

$$Q = 1, 1 - \frac{2p(z-1) - 2}{p(z-1)(z-2)} \tag{4.29}$$

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

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p\left(1 - \left(\frac{1-p}{p}\right)^3\right) & \text{for } p \geq p_c \end{cases} \tag{4.30}$$

Let,

$$f(p) = \left(\frac{(1-p)}{p}\right)^3 \tag{4.31}$$

Then

$$f'(p) = -3p^-4(1-p)^3 - 3p^-3(1-p)^2$$
$$= -\frac{3}{p}\left(\frac{(1-p)}{p}\right)^3 - \frac{3}{p}\left(\frac{(1-p)}{p}\right)^2 \tag{4.32}$$

$$P(p) = P(p_c) + (p - p_c)P'(p_c) + \ldots \tag{4.33}$$
$$= 0 + (p - p_c)\left(1 - f(p_c) - pf'(p_c)\right) + \ldots \tag{4.34}$$
$$= 6(p - p_c) + \ldots \tag{4.35}$$
$$\tag{4.36}$$

Therefore we get

$$P(p) \propto (p - p_c) \text{ for} p \to p_c^+ \tag{4.37}$$

the critical exponent β is defined by

$$P(p) \propto (p - p_c)^\beta \tag{4.38}$$

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,

$$T = (1 - p) \times 0 + p(1 + 2T) \tag{4.39}$$

Solving this we get

$$T = \frac{p}{1 - 2p} \tag{4.40}$$

for $p < p_c$.

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

$$S(p) = 1 + 3T \tag{4.41}$$
$$= \frac{1 + p}{1 - 2p}$$
$$= \frac{1 + p}{2(p_c - p)}$$
$$= \frac{1 + p}{2}(p_c - p)^{-1} \tag{4.42}$$

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

$$g(r) = z(z-1)^{r-1}p^r \tag{4.43}$$
$$= \frac{z}{z-1}(p(z-1))^r \tag{4.44}$$
$$= \frac{z}{z-1}\exp\left[\log\left[p(z-1)\right]\right] \tag{4.45}$$

The value of percolation threshold for Bethe lattice can be found by analyzing the behaviour of the correlation function at large distances, i.e. at r $\rightarrow \infty$. For $p(z-1) < 1$, $g(r)$ decreases exponentially, on the other hand for $p(z-1) > 1$, the correlation function diverges which signifies the existence of an infinite cluster. Mathematical treatment yields the correlation length from 4.6

$$\begin{aligned}
\xi &= \frac{-1}{\log[p(1-z)]} \\
&= \frac{-1}{\log(p/p_c)} \\
&= (p - p_c)^{-1}
\end{aligned} \tag{4.46}$$

as p approaches p_c, that is $\nu = 1$.

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.

4.6 Relation of Phase Transition with Percolation

4.7 Application

Definitions of some quantities used in percolation. Basic Algorithm

4.7.1 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 $L = \{L_1, L_2, \dots L_n\}$, where n is a finite number and $L_1 < L_2 < \dots < L_n$), and extrapolate the results for infinite lattice. The visual structure of the square lattice is as follows 4.4. This is and empty lattice structure. Filled circles are for occupied site and filled bonds are for occupied bonds 4.5.
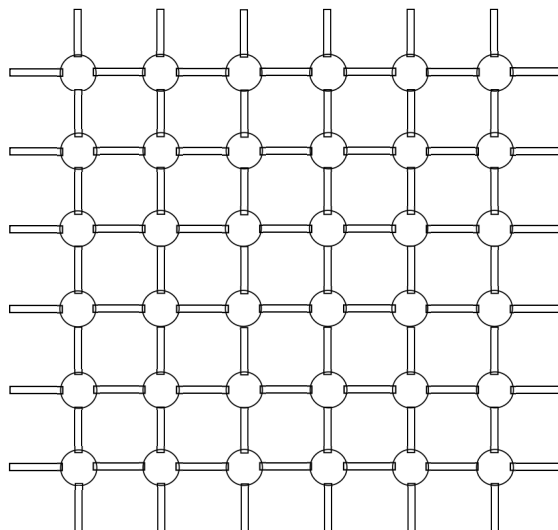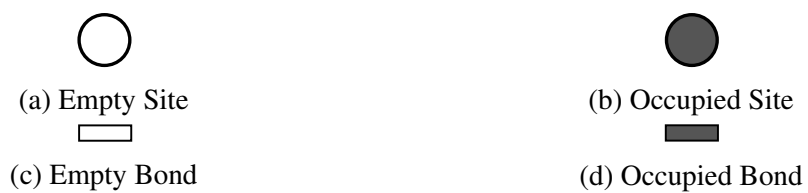
Fig. 4.4 Square Lattie (empty) of length 6

(a) Empty Site   (b) Occupied Site

(c) Empty Bond   (d) Occupied Bond

Fig. 4.5 Site and Bond symbol (empty and occupied).

4.7.2   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.

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 4.6.

4.7.3   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.

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 4.7.

(a) Initial state

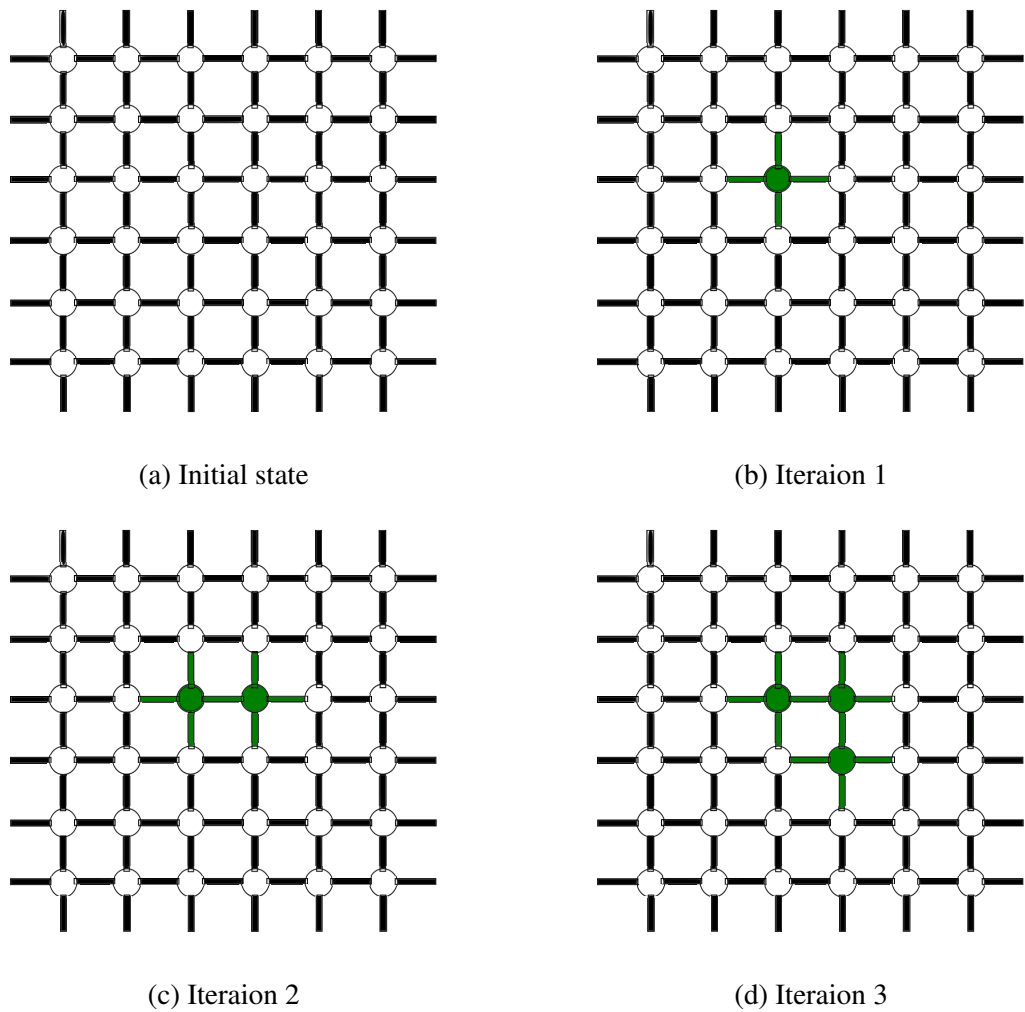(b) Iteraion 1

(c) Iteraion 2

(d) Iteraion 3

Fig. 4.6 Growth of a Cluster in Site Percolation on square Lattice

(a) Initial state

(b) Iteraion 1

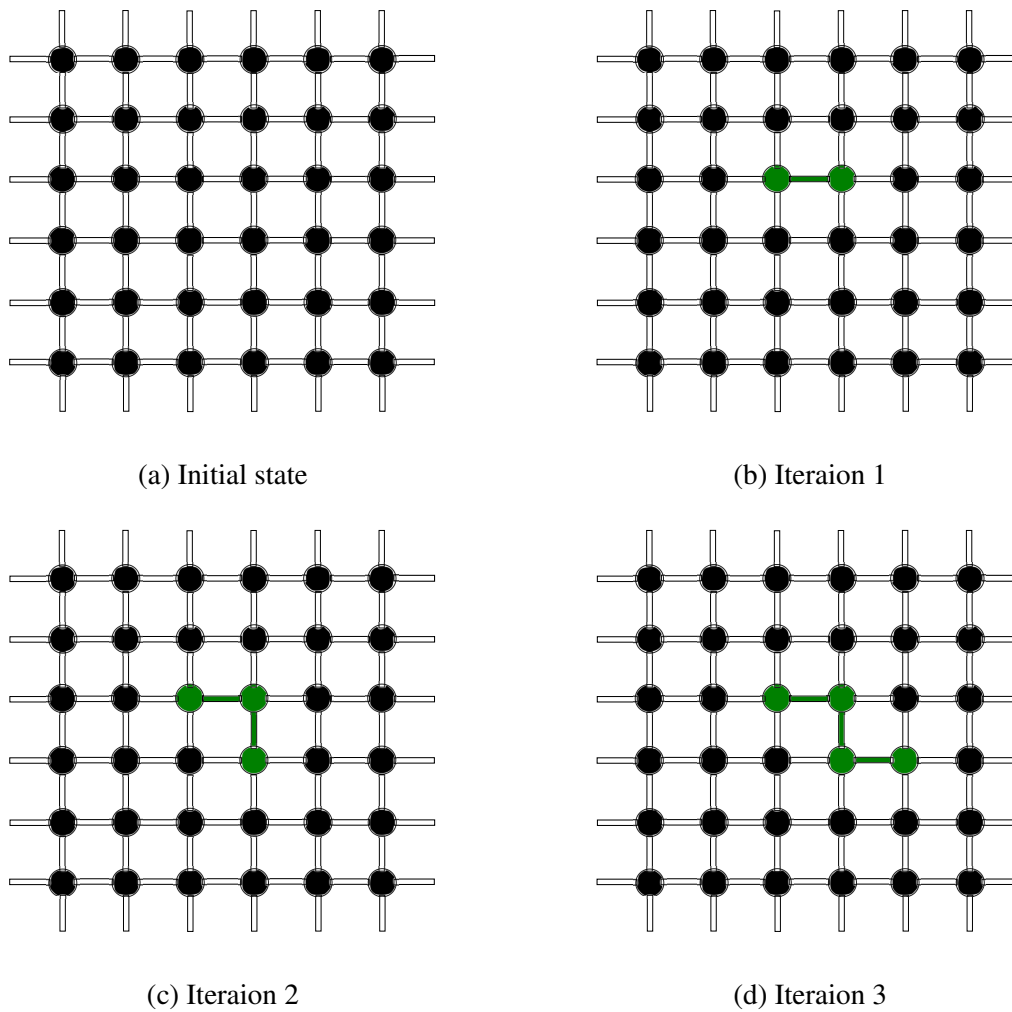(c) Iteraion 2

(d) Iteraion 3

Fig. 4.7 Growth of a Cluster in Bond Percolation on square Lattice

4.8   Definitions

4.8.1   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 [20]. 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.

4.8.2   Order Parameter

Percolation strength or P is defined as to 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. In a system where spanning cluster does not make any sense, the largest cluster is used instead of the spanning cluster. Examples of such system are Network and Bethe Lattice. Mathematically

$$P(p,L) = \frac{K}{\sum_i k_i} \tag{4.47}$$

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. But when simulating the program, performing summation as in the denominator of equation 4.47 is time consuming. But since we know that the sum is always a constant and it is $2L^2$ for a square lattice in periodic boundary condition. Hence we write

$$P(p,L) = \frac{K}{2L^2} \tag{4.48}$$

4.8.3   Entropy

Entropy or Shanon Entropy is defined as

$$H = \sum_i -\mu_i \log(\mu_i) \tag{4.49}$$

where μ_i is the probability that the randomly picked site will belong to the $i-th$ cluster. Mathematically

$$\mu_i = \frac{k_i}{\sum_i k_i} \tag{4.50}$$

where k_i is the size of the $i-th$ cluster. Entropy is the measure of disorderedness of a system.

Occupation Probability

$$(p - p_c) \sim L^{-1/\nu} \tag{4.51}$$
$$\log(p - p_c) \sim -1/\nu \log(L) \tag{4.52}$$

Specific Heat

$$C \sim L^{\alpha/\nu} \tag{4.53}$$
$$\log(C) \sim \alpha/\nu \log(L) \tag{4.54}$$

Order Parameter

$$P \sim L^{-\beta/\nu} \tag{4.55}$$
$$\log(P) \sim -\beta/\nu \log(L) \tag{4.56}$$

Susceptibility

$$\chi \sim L^{\gamma/\nu} \tag{4.57}$$
$$\log(\chi) \sim \gamma/\nu \log(L) \tag{4.58}$$

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 $n_s(p_c) \sim s^{-\tau}$ 4.4.8 and the fractal dimension d_f that characterizes the spanning cluster at p_c 4.4.11. 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   Building The Structure

5.2   Percolation Algorithm

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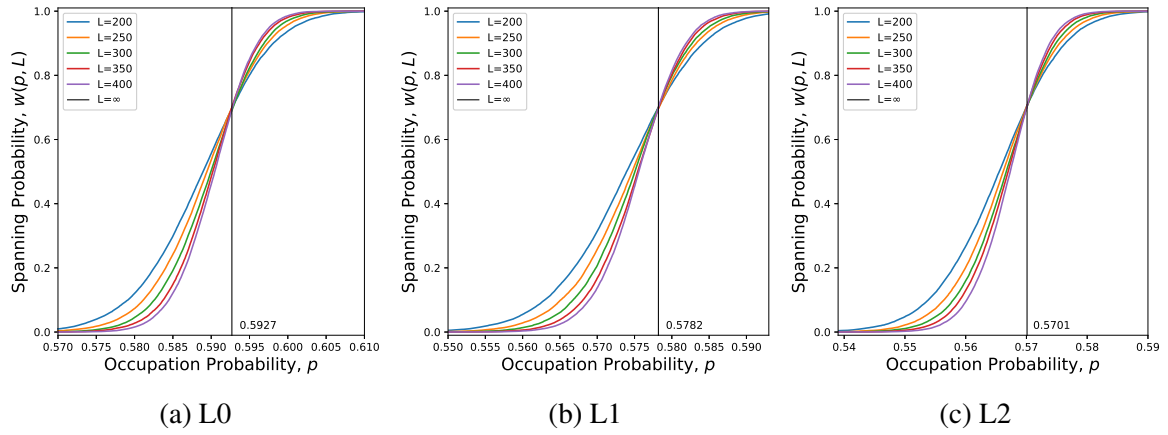
Fig. 5.1 Spanning Probability, $w(p, L)$ vs Occupation Probability, p

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 $1/\nu$

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 $1/\nu$. If we now use the finite size scaling (FSS) hypothesis
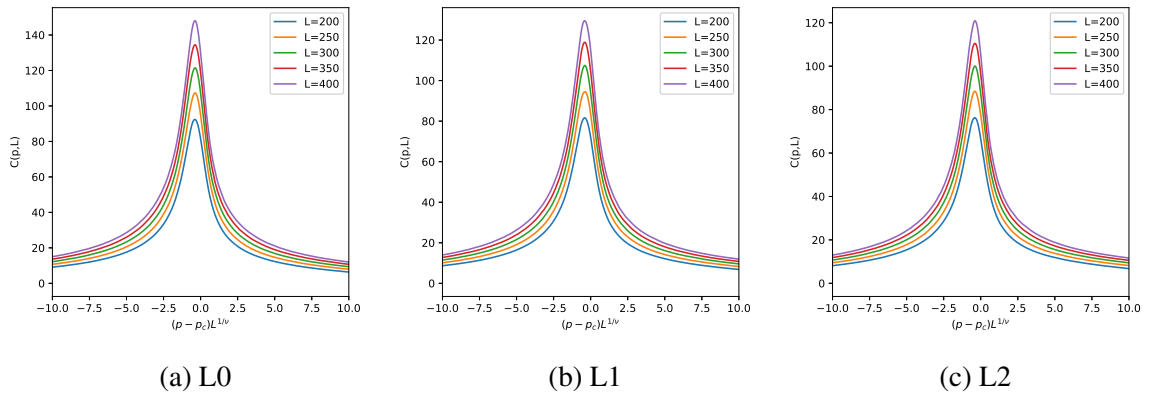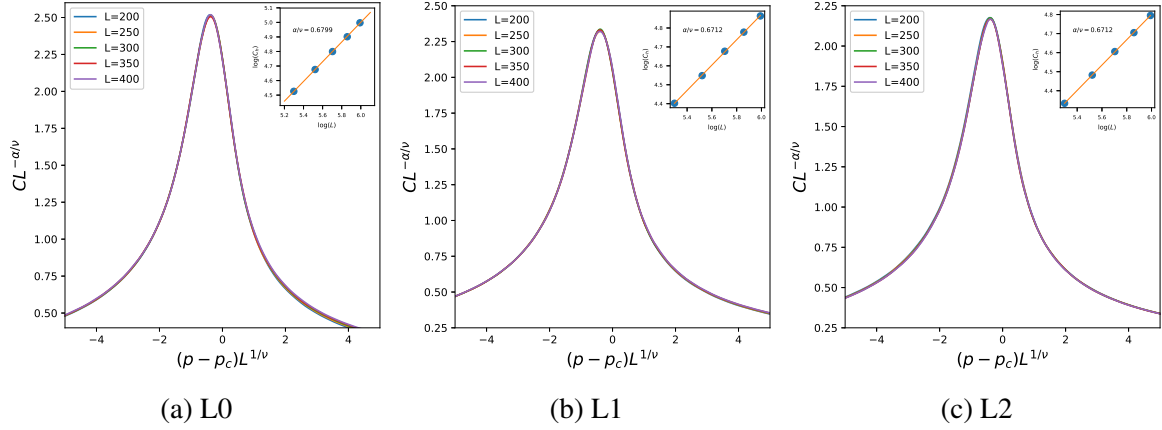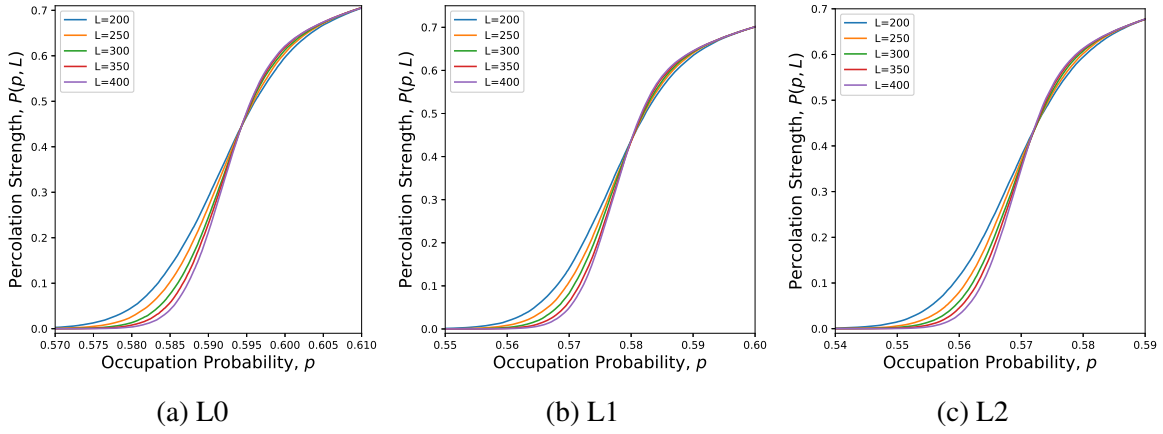
$$w = (p - p_c)L^{1/\nu} \tag{5.1}$$

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

(a) L0 (b) L1 (c) L2

Fig. 5.2 $w(p,L)$ vs $(p-p_c)L^{1/\nu}$

(a) L0 (b) L1 (c) L2
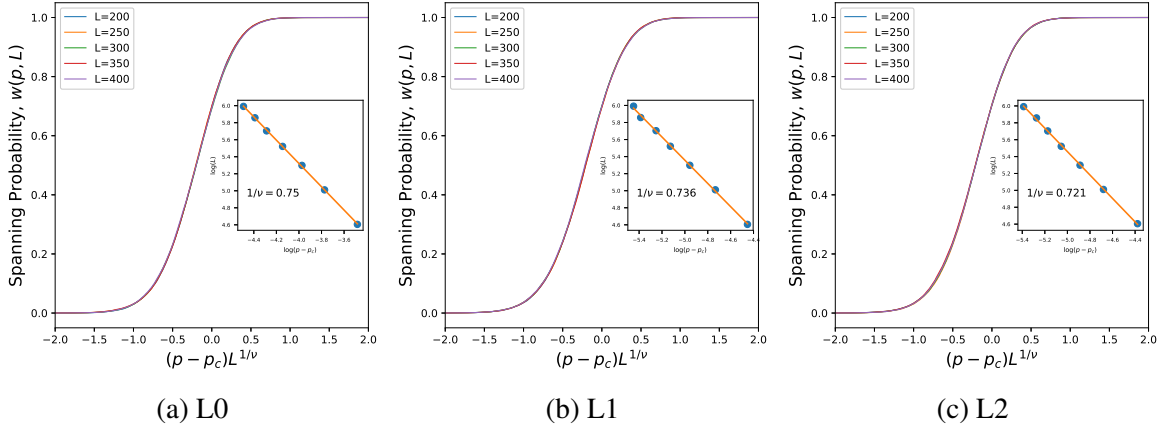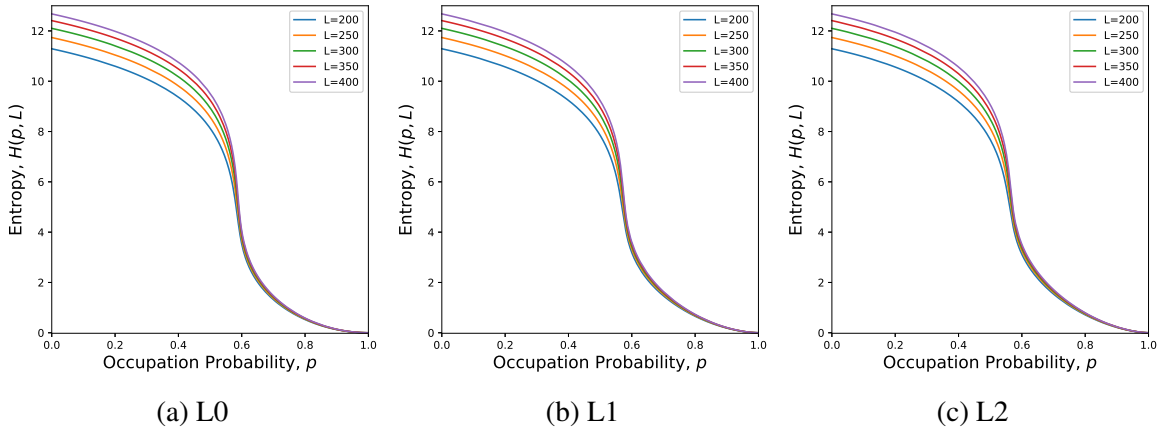
Fig. 5.3 Entropy, $H(p,L)$ vs Occupation Probability, p

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 [22]. Using the definition **??** 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 $1/\nu$ obtained from 5.4.2 and get the graph as in 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 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

(a) L0   (b) L1   (c) L2
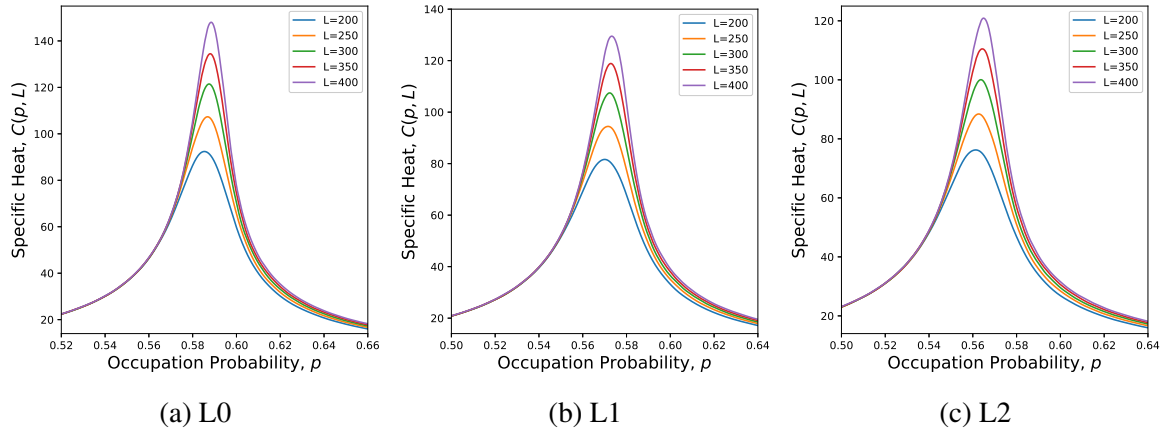
Fig. 5.4 Specific Heat, $C(p, L)$ vs Occupation Probability, p

(a) L0   (b) L1   (c) L2

Fig. 5.5 $C(p, L)$ vs $(p - p_c)L^{1/\nu}$

(a) L0   (b) L1   (c) L2

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

(a) L0   (b) L1   (c) L2

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

$(p - p_c)L^{1/\nu}$ 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 4.48 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 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

(a) L0   (b) L1   (c) L2
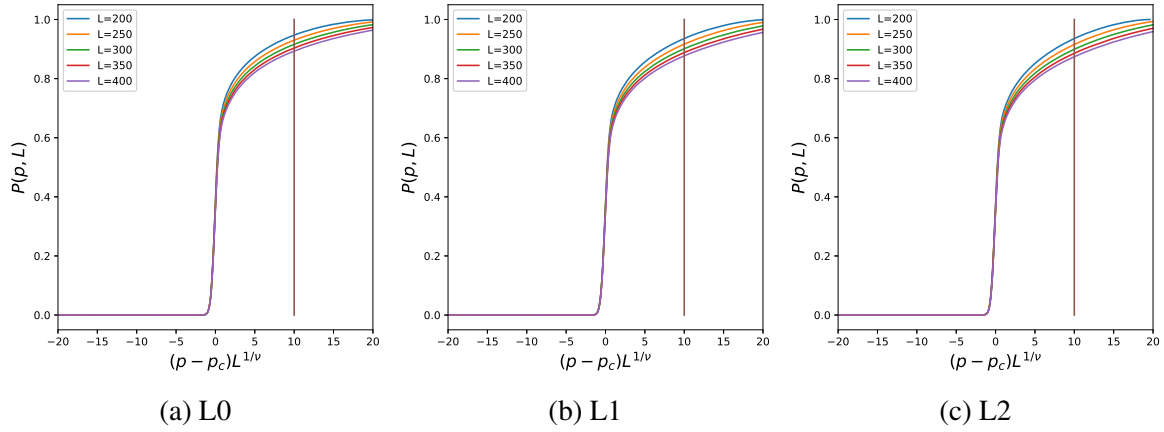
Fig. 5.8 Order Parameter, $P(p,L)$ vs Occupation Probability, p

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

(a) L0   (b) L1   (c) L2
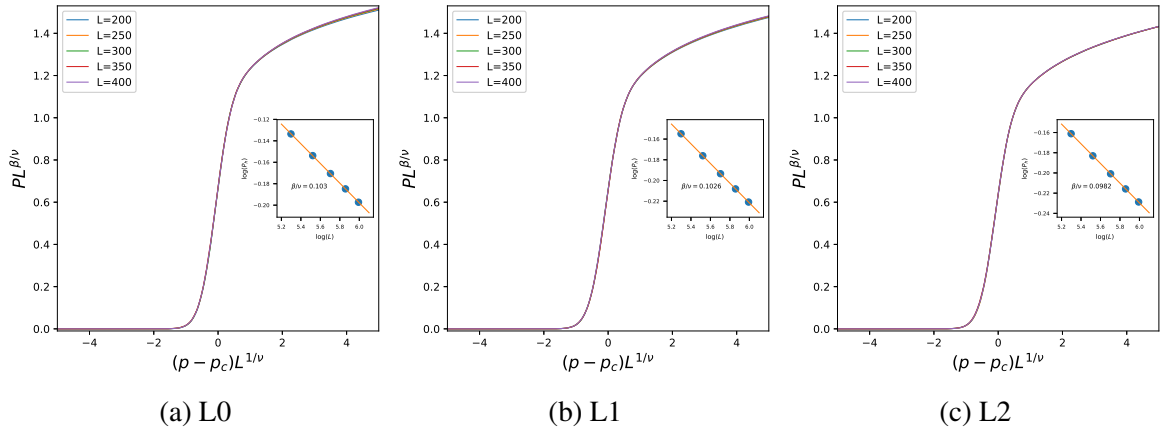
Fig. 5.10 $PL^{\beta/\nu}$ vs $(p-p_c)L^{1/\nu}$

get the exponent β/ν from it's slope and obtain exponent β by dividing β/ν by $1/\nu$. Using the FSS hypothesis **??** 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 aligned (figure 5.12). Note that the value of $1/\nu$ 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/ν. And using the FSS hypothesis

(a) L0   (b) L1   (c) L2
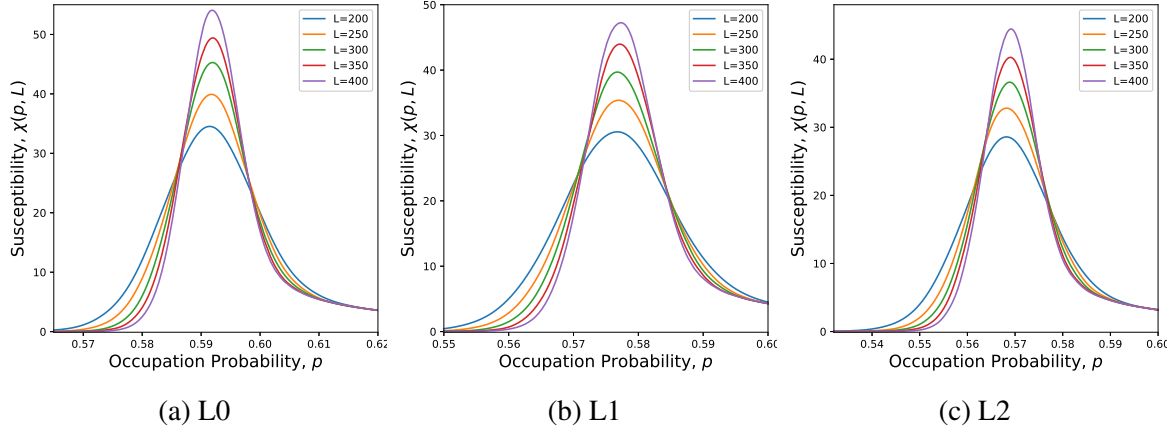
Fig. 5.11 Susceptibility, $\chi(p,L)$ vs Occupation Probability, p

(a) L0   (b) L1   (c) L2
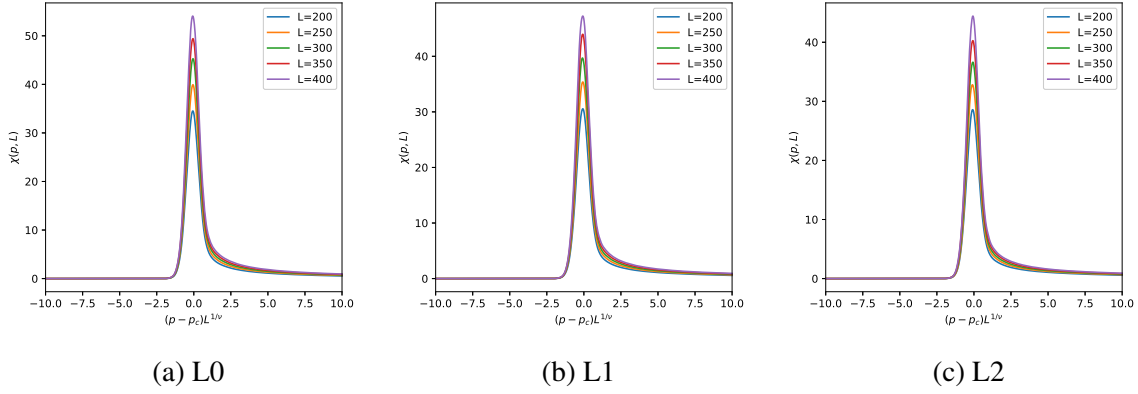
Fig. 5.12 $\chi(p,L)$ vs $(p - p_c)L^{1/\nu}$

we plot $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ and obtain a perfect data collapse. It is shown in figure 5.13. 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

### 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

(a) L0   (b) L1   (c) L2
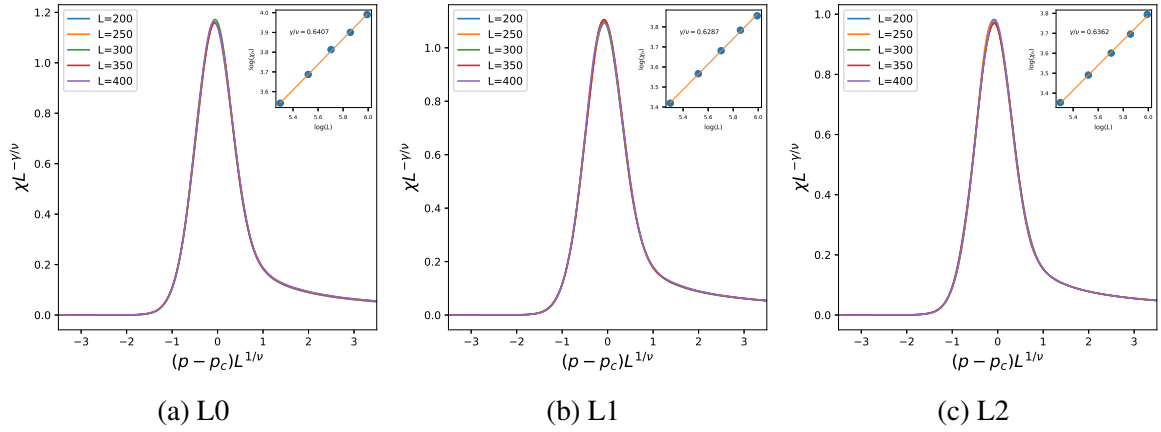
Fig. 5.13 $\chi L^{\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$

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

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

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

(a) L0   (b) L1   (c) L2
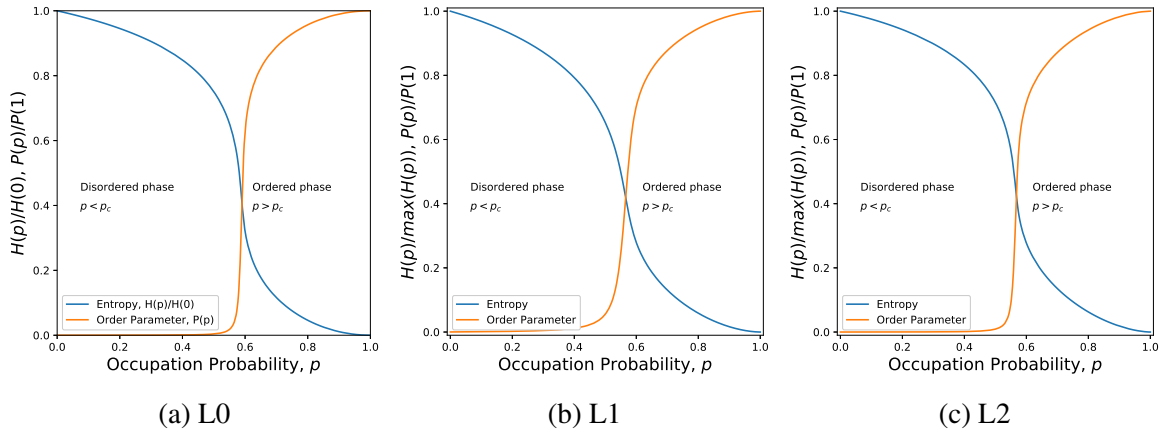
Fig. 5.16 $H(p,L)/H(0,L)$ or $P(p,L)/P(1,L)$ vs p

(a) L0   (b) L1   (c) L2
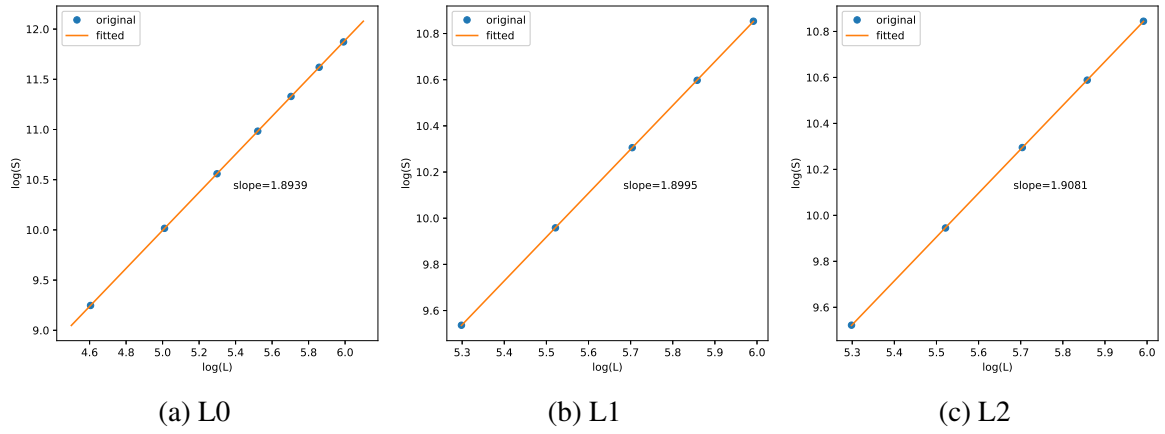
Fig. 5.17 $\log(S)$ vs $\log(L)$

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.

Chapter 6

Summary and Discussion

Up until now we knew the exponents for $L0$ or direct interaction. We have investigated for short and long range interactions and we call this $L1$ and $L2$ respectively. Where $L1$ 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 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.

Interaction	p_c	$1/v$	α/v	β/v	γ/v
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	$1/\nu$	α	β	γ	$\alpha + 2\beta + \gamma$	d_f
L0	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

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Appendix A

Percolation

A.1 Algorithm

A.2 Code

Complete code for percolation on square lattice is available at https://github.com/sha314/SqLatticePercolation

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 $1/\nu$. The critical point is denoted as x_c To find an estimate from the data that looks like the graph of specific heat or susceptibility, the following algorithm is very helpful

1. get the x and y values of the convoluted data for all lengths (L)

2. get the x value at a specific height, h, and call it x_h

3. plot a graph of $log(|x_h - x_c|)$ vs $log(L)$ where $||$ denotes the absolute value.

4. slope of this graph is the estimate for the exponent $1/\nu$

Now to find the exponent that best collapses the data is the main goal. To do this the following algorithm can be followed.
Finding the standard deviation of the points at height h after scaling x-values with an approximate value of the exponent $(1/nu)_{approx}$ that is obtained from the graph of $log(|x_h - x_c|)$ vs $log(L)$.

1. write a function that takes h, x_{scaler}, y_{scaler}, lr as argument where, h is the height at which we will be taking x-values, x_{scaler} is the exponent that scales the x-values, y_{scaler} is the exponent that scales the y-values and lr is the argument that tells if the left or right side of the critical point should be taken under consideration. call this function *find_x_deviation*
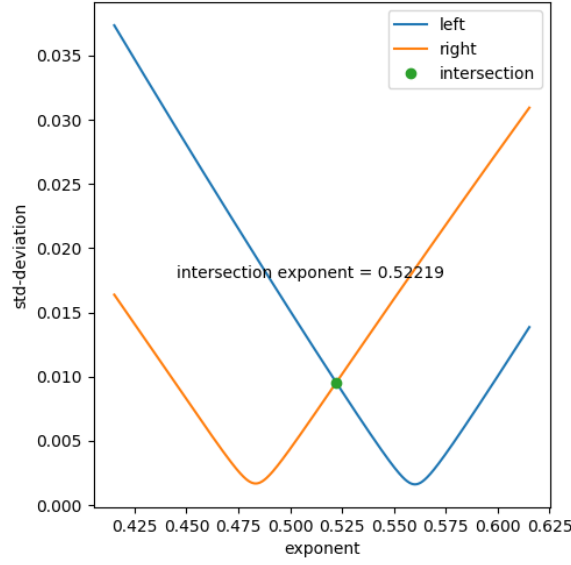
Fig. C.1 Best collapsing on either right or left
??

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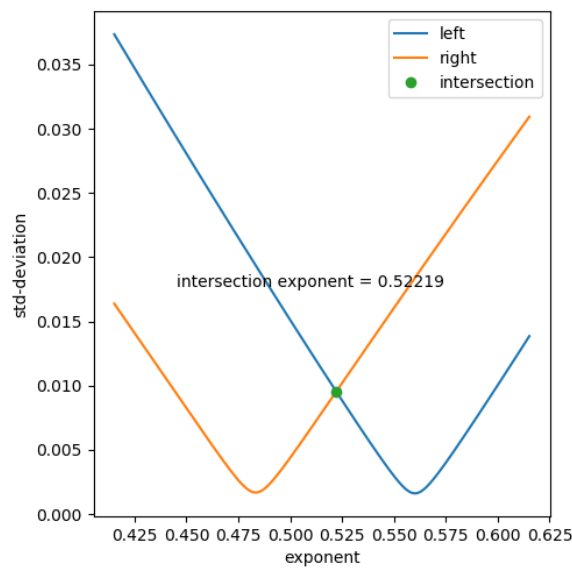
Fig. C.2 Minimizing exponent for scaling *x*-values

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.