Polydispersity Effect and Universality of Finite-Size Scaling Function

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We derive an equation for the existence probability $E_p$ for general percolation problem using an analytical argument based on exponential-decay behaviour of spatial correlation function. It is shown that the finite-size scaling function is well approximated by the error function. The present argument explain why it is universal. We use Monte Carlo simulation to calculate $E_p$ for polydisperse continuum percolation and find that mono- and polydisperse system have the same finite-size scaling function.

KEYWORDS: continuum percolation, universal finite-size scaling function, size dispersity

§1. Introduction

Percolation is fundamental in science.1, 2 It shows many interesting phenomena including phase transitions. One of its most interesting features is scaling. According to finite-size scaling theory,2, 3 the existence probability $E_p$, which is defined as the probability that the system percolates, has the form

$$E_p(L, ho) = F((\rho - \rho_c)L^{1/\nu}),$$

where $\rho$, $\rho_c$, $L$, and $\nu$ are density, critical density, the linear size, and the critical exponent of correlation length, respectively. It has been found that not only the exponents but also the function $F$ is universal for bond, site and continuum percolation models in the same spatial dimensions.4-6 Therefore, $F$ is called the universal finite-size scaling function (UFSSF). The universality of critical exponents has been studied well, and UFSSF is actively studied in recent years.7

In the present paper, we consider that why the finite-size scaling function shows universality and derive an expression of $E_p$. We confirm the expression of $E_p$ derived in the following reproduces the results from computer simulation well. We also study polydisperse continuum percolation model (CPM) to see the effect of polydispersity on the universality of the finite-size scaling function. Although polydispersity effect modifies the fluid-solid transition,8-11 in this paper we find that the systems with mono- and polydispersity have the same finite-size scaling function for their $E_p$.

§2. Derivation of $E_p$

2.1 Correlation function

The function to express the existence probability $E_p$ must be derived from some feature which are independent of percolation types, because finite-size scaling function is observed to be independent of percolation models. Therefore we treat asymptotic behaviour of a correlation function $X(r)$. In the case of percolation models, the correlation function is the probability that two particles(or sites) at a distance $r$ are in the same cluster. Near the critical point, the correlation length $\xi$ is written as

$$\xi = B|\rho - \rho_c|^{-\nu},$$

where $B$, $\rho$, $\rho_c$ and $\nu$ are proportional constant, density, critical density and the critical exponent of correlation length, respectively. Correlation function $X(r)$ is approximated as

$$X(r) = A \exp(-r/\xi),$$

with a constant $A$ for large $r$ when $\rho < \rho_c$. We will derive the existence probability $E_p$ with using this $X(r)$.

2.2 Free boundary condition

Consider a general two dimensional percolation problem that a square box of the size of $L \times L$ is occupied by particles with density $\rho$. The system is assumed to have free boundary and the Cartesian coordinates are taken. The probability that a particle in $(x, 0)$ and a particle in $(y, L)$ are both in the same cluster will be expected to be proportional to $\exp(-\sqrt{L^2 + (x - y)^2}/\xi)$. The probability that the top and the bottom of the system is in the same cluster, that is, the existence probability $E_p$ will be approximately given by

$$E_p = \frac{C}{L^2} \int_0^L \int_0^L \int_0^L \int_0^L \exp \left( -\frac{L}{\xi} \sqrt{1 + (x - y)^2}/L^2 \right),$$

with an arbitrary constant $C$. Note that we neglect many-point correlation and assume the correlation length is a simple exponential function. The validity of this theory is confirmed by computer simulation later.

Equation (2.3) can be simplified by substituting $u = (x + y)/L$ and $v = (x - y)/L$, and by using the saddle-point approximation with $\sqrt{1 + v^2} \simeq 1 + v^2/2$. Then
eq. (2.3) is reduced to
\[ E_p = C e^{-L/\xi} \int_{-1}^{1} dv \exp \left( -\frac{L}{2\xi} v^2 \right) \]
\[ = C e^{-L/\xi} \sqrt{\frac{\pi \xi}{L}} \left( \text{erf} \left( \sqrt{L/2\xi} \right) - \text{erf} \left( -\sqrt{L/2\xi} \right) \right). \]
\[ (2.4) \]
\[ (2.5) \]
Near the critical point, \( \xi \approx L \), we can express the existence probability with the error function,
\[ E_p(L, \rho) = C e^{-L/\xi} \sqrt{\frac{\pi \xi}{L}} \text{erf} \left( \sqrt{\frac{L}{2\xi}} \right). \]
\[ (2.6) \]
This \( E_p \) is the function of \( L/\xi \), or \( (L/\xi)^{1/\nu} = B^{-1/\nu} |\rho - \rho_c|^{1/\nu}. \) So it is the form of eq. (1.1). The constant \( C \) is defined by \( E_p(L, \rho_c) = 1/2 \) for example.

The parameter \( B \) in eq. (2.1) is an index of easiness to connect locally, and is independent of the boundary condition and shape of boundary. It depends on type of percolation models, so it is not an universal parameter. Once we have the parameter, we can calculate \( E_p \). But it is difficult to get the correlation function of the system and calculate \( E_p \) precisely. So let us introduce another parameter named \( a \) in the next section.

### 2.3 Other boundary conditions

Above argument treats the case of the square system with free boundary condition. In this subsection, we try to extend the theory for non-square system and other boundary conditions.

First, we consider a rectangular boundary with general aspect ratio. In this case, eq. (2.6) should be modified, because it considers the probability that there is only one percolating cluster in the system. For the aspect ratio \( L_2/L_1 = 1 \) with a linear dimension \( L_1 \) in the horizontal direction and \( L_2 \) in the vertical direction, the probability that the system percolates with many clusters will be negligible. But with the general aspect ratio, we have to consider such configurations if \( L_2/L_1 < 1 \). In this case, a probability \( 1 - E_p \) that the system does not percolate is written with the correlation function \( X(r) \) as,
\[ (1 - E_p) = \prod_{x=0}^{L_1} \prod_{y=0}^{L_1} \left[ 1 - X \left( \sqrt{L_2^2 + (x-y)^2} \right) \right]. \]
\[ (2.7) \]
With eq. (2.2), this is approximated as
\[ (1 - E_p) \]
\[ = \prod_{x=0}^{L_1} \prod_{y=0}^{L_1} \left( 1 - \frac{C}{L_1 L_2} \exp \left( \frac{L_2}{\xi} \sqrt{1 + (x-y)^2/L_2^2} \right) \right), \]
\[ (2.8) \]
where \( E_p \) is the probability there is at least one cluster which reaches from the horizontal side to the other horizontal side of the system and \( C \) is a constant.

With the saddle-point approximation as used when eq. (2.6) is derived, we have
\[ \log (1 - E_p) = -C e^{-L_2/\xi} \int_{-L_1/L_2}^{L_1/L_2} dv \exp \left( -\frac{L_2}{2\xi} v^2 \right) \]
\[ \approx -C e^{-L_2/\xi} \sqrt{\frac{\pi \xi}{2L_2}} \text{erf} \left( \sqrt{\frac{L_1^2}{2\xi L_2}} \right). \]
\[ (2.9) \]
So we have the following expression of \( E_p \),
\[ E_p = 1 - e^{-f(L_1, L_2, \xi)}, \]
\[ (2.10) \]
with
\[ f(L_1, L_2, \xi) = C e^{-L_2/\xi} \sqrt{\frac{\pi \xi}{2L_2}} \text{erf} \left( \sqrt{\frac{L_1^2}{2\xi L_2}} \right). \]
\[ (2.11) \]
Equation (2.10) is reduced to
\[ E_p = f(L_1, L_2, \xi) \]
\[ = C e^{-L_2/\xi} \sqrt{\frac{\pi \xi}{2L_2}} \text{erf} \left( \sqrt{\frac{L_1^2}{2\xi L_2}} \right) \]
\[ (2.12) \]
with approximation \( e^{-t} \approx 1 - t \) when \( t \ll 1 \). The existence probability of the system with general aspect ratio is also written as the error function. When aspect ratio \( L_1/L_2 = 1 \), eq. (2.12) reduces the eq. (2.6).

Next, we consider the square system with periodic boundary condition vertical direction to the percolation direction. We can calculate the existence probability of the square periodic system with neglecting long distance correlation, and the \( E_p \) is written as
\[ E_p = \frac{C}{L^2} \int_0^L \int_{-L/2}^{L/2} dx \exp \left( -\frac{L}{\xi} \sqrt{1 + v^2/L^2} \right) \]
\[ (2.13) \]
with a constant \( C \). The constant \( C \) is defined by \( E_p(L, \rho_c) = 1/2 \) like as free-boundary case. Equation (2.13) is derived by noting that all points at the bottom of system are equivalent because of the periodic boundary condition, so the equation becomes simpler than the free-boundary case. We can evaluate eq. (2.13) with similar discussion of free boundary case. By substituting \( u = x/L \), and by using the saddle-point approximation with \( \sqrt{1 + v^2} \approx 1 + v^2/2 \), eq. (2.13) is reduced to
\[ E_p = \frac{C}{4} e^{-L/\xi} \int_{-1}^{1} dv \exp \left( -\frac{L}{2 \xi} v^2 \right) \]
\[ \approx C' e^{-L/\xi} \sqrt{\frac{\pi \xi}{2L}} \text{erf} \left( \sqrt{\frac{L}{2\xi}} \right). \]
\[ (2.14) \]
\[ (2.15) \]
It means that there is also universal finite-size scaling function for periodic boundary cases.

### §3. Simulation

#### 3.1 Scaling of two different percolation systems

The theory in the previous section is verified by using the computer simulation. First of all a new parameter which is useful to compare and to make scaling analysis of two models X and Y is introduced. These models X and Y are assumed to have the same correlation-length
exponent. It is denoted by $\alpha$ defined by,

$$\alpha = \left( \frac{B_X}{B_Y} \right)^{-1/\nu},$$

where $B_X$ and $B_Y$ are the correlation-length amplitudes (see eq. (2.1)).

If the scaling function (2.6) is reproduced when the scaled densities are taken to be

$$\rho'_X = \left( \frac{L}{\xi_X} \right)^{1/\nu} = C_X (\rho - \rho_c^X) L^{1/\nu}$$

and

$$\rho'_Y = \left( \frac{L}{\xi_Y} \right)^{1/\nu} = C_Y (\rho - \rho_c^Y) L^{1/\nu},$$

the parameter $\alpha$ is expressed as

$$\alpha = \frac{C_X}{C_Y},$$

because $C_X = B_X^{-1/\nu}$ and $C_Y = B_Y^{-1/\nu}$.

Consider the two boundary conditions, for example, free and periodic boundary conditions. For different boundary conditions, a system has different form of $E_p$. But we can scale two models of the periodic boundary condition and free boundary case with the same $\alpha$, because the $\alpha$ only depends on the correlation-length amplitudes which are expected to be independent of the boundary conditions.

With similar argument, $\alpha$ is universal even if the shape of boundary is changed. Generally, $\alpha$ is independent of boundary.

So far, we have seen the origin of the universality of finite-size scaling function with using the general feature of correlation function, and define new parameter $\alpha$ which is expected to be independent of boundary condition of the system. We try to compare the derived $E_p$ and calculated $E_p$ with simulation in the following subsection.

### 3.2 Simulated results and calculated $E_p$

Here, we treat bond and site percolation models. Each bonds and sites are occupied with the probability $p$ in a square on rectangular lattice. Two sites are considered to be in the same cluster when two occupied sites are in the neighbourhood or the bond between two sites are occupied. If there is a cluster which stretches from the top to the bottom of the system, the system percolates. Free and periodic boundary cases are studied. We use Monte Carlo method to calculate $E_p$. 50000 independent simulations are averaged at each density.

Figure 1 shows fitting results the $E_p$ of the bond percolation models and eq. (2.3). The system size $L$ are 32, 64, 128. The only arbitrary fitting parameter is $B$, the proportional constant of correlation length to density. It shows good coincidence except for the system size 32, because the assumption that the correlation length decays as simple exponential is not good for the small system. Equation (2.3) is valid only smaller density than $\rho_c$, but interesting thing is we can fit $E_p$ and the simple error function at every density. Figure 2 shows fitting results that the error function and $E_p$ of site percolation model (SPM) and bond percolation model (BPM). The system size $L$ is 128. The scaled $E_p$ is shown as Fig. 3. We use the value of $\alpha = 1.26 \pm 0.02$ to scale $E_p$ of SPM and BPM.

Figure 4 shows scaled $E_p$ of SPM and BPM with periodic boundary condition. In this case, $\alpha = 1.20 \pm 0.02$.

We also consider non-square system. Figure 5 shows that scaled $E_p$ of SPM and BPM, the system size is $128 \times 128$. Fig. 1. Estimated values of existence probability $E_p$ of site percolation model in square boxes is plotted as a function of $s = (\rho - \rho_c)$ and fit results using eq. (2.6) (lines). The system sizes are 32×32, 64×64 and 128×128. Fig. 2. Estimated values of existence probability $E_p$ of site, bond and continuum percolation in square boxes of the site of 128×128 and fitting results with the error function are shown as a function of density $\rho$. Error bars are smaller than marks. Fig. 3. Existence probabilities of SPM and BPM systems are plotted as a function of scaled density. The system size is $128 \times 128$. Fig. 4. Existence probability $E_p$ of SPM and BPM with periodic boundary conditions. Fig. 5. Existence probability $E_p$ of SPM and BPM with non-square system.
Fig. 4. Existence probabilities of SPM and BPM systems with periodic boundary condition are plotted as a function of scaled density. The system size is $128 \times 128$.

Fig. 5. Existence probabilities of SPM and BPM systems with non-square boundary are plotted as a function of scaled density. The system size is $128 \times 64$.

64. We find the value of $\alpha$ is $1.27 \pm 0.02$ in this case. We can confirm that the value of $\alpha$ is almost universal for free boundary cases. As for the periodic case, $\alpha$ is slight different from free boundary cases. The assumption may not valid that correlation length of the systems with free and periodic boundary have the same behaviour.

§4. Polydispersity Effect for Universality of Finite-Size Scaling Function

4.1 Size dispersity and scaling behaviour

The scaling behaviour is interpreted to be caused by the fact that the system only depends on $L/\xi$ with the system size $L$ and the correlation length $\xi$. We are interested in whether the system with monodisperse and polydisperse particles have the same UFSSF. We consider the case when the system has size dispersion. In other words, more degree of freedom are introduced to the system in addition to $L/\xi$, it may break the universality. To consider this problem, we study continuum percolation model (CPM) with size dispersity.

4.2 Monodisperse continuum percolation model

First, we confirm the behaviour of the monodisperse model. N disks of identical radius are randomly put in a $L \times L$ square box. The disks are soft and may overlap without any constraints. Two disks are considered to be in the same cluster if and only if they overlap; this is the system of soft disks studied by Hu and Wang.\(^6\)

The density $\rho$ of disks is defined by $\rho = N \pi r^2 / L^2$, where $N, r$ are the number of the disks and the radius of the disks, respectively. The disks’ radius $r$ is selected to be $\sqrt{2}/2$ to optimise the calculation. If there is a cluster which stretches from the top to the bottom of the box, the system percolates. We use Monte Carlo method to calculate the existence probability $E_p(L, \rho)$ for systems with free boundary conditions and $L = 64, 80, 128$.

The typical configuration is shown as Fig. 6. 50,000 independent simulations are averaged at each density and the results are presented in Fig. 7. The existence probability with scaled density $\rho' = (\rho - \rho_c)L^{1/\nu}$ is given in Fig. 8. The value of $\nu$ is selected to be $\nu = 4/3$ for two dimensional percolation.\(^2\) It is confirmed by fitting in the simulation and it is expected from the universality of the exponent. Here instead of $\rho_c$, the effective critical density $\rho_c(L)$ defined by $E_p(L, \rho_c(L)) = 0.5$ is used to make the following analysis simple. This $\rho_c(L)$ is the density when the correlation length $\xi$ becomes of the order of the system size $L$. Thus the $\rho_c(L)$ has $L$ dependence like $\rho_c(L) = \rho_c + AL^{-1/\nu}$ with a constant $A$. This equation is also written as following expression,

$$(\rho - \rho_c(L))L^{1/\nu} = (\rho - \rho_c)L^{1/\nu} + A.$$  

Therefore the difference between using $\rho_c$ and using $\rho_c(L)$ is a translation in the scaling variable. Figure 8 shows a good scaling behaviour.

4.3 Polydisperse system

We consider CPM with polydispersity as following. The existence probability for systems with size dispersity is calculated like in the monodisperse case. Two kinds of disks are put in a square box randomly, permitting overlap. The density $\rho$ is defined by $\rho = \pi \sum_{i=1}^N r_i^2 / L^2$. The disks have two kinds of radius; $N/2$ disks have a radius $r = \sqrt{2}/2$, and the other has the radius $r = 1/2$. This system is bi-disperse. The dispersity $\sigma^2$ of the system measured by $\sigma^2 = \frac{\langle (\Delta r)^2 \rangle}{\langle r_i^2 \rangle^2} = \frac{\langle r_i^2 \rangle}{\langle r_i^2 \rangle} - 1 \approx 0.029$, \(^7\)}
which is much larger than the characteristic dispersity $\sigma^2 = 0.0073(5)$ above which the co-existence-like intermediate phase of fluid-solid transition vanishes for hard-disk system. So if polydispersity changes the universality of UFSSF, the value of dispersity may be large enough. The values of existence probability $E_p(\rho)$ are calculated by Monte Carlo simulations; 50,000 independent simulations are averaged at each density. The typical configuration of bi-disperse system is shown as Fig. 9.

The calculated values of $E_p(\rho)$ are given in Fig. 10, and is given in Fig. 11 with scaled density $\rho' = (\rho - \rho_c)L^{1/\nu}$. The $\rho_c(L)$ is defined as in the monodisperse case. Comparison between the monodisperse and the bi-disperse cases is given in Fig. 12 which shows that the results for mono- and bi-disperse percolation fall on the same curve. So the two systems have the same scaling function.

§5. Summary and Discussion

In this paper, we presented a general theory for the critical phenomena, especially for the UFSSF of percolation phenomena. We showed that the existence probability is approximately written with the error function, and confirmed it reproduce the simulation results well.

We derived the existence probability with using the correlation function. It means $E_p$, the macroscopic value, is given by integrating the correlation function, the microscopic value. The identity of the system, for example, type of system (such as SPM, BPM and CPM) or type of grid (like as triangular, square and honeycomb lattice), is represented by the only one parameter $B$. These

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**Fig. 7.** Estimated values of existence probability $E_p$ of monodisperse continuum percolation in square boxes of the site of $64 \times 64, 80 \times 80, 128 \times 128$ are shown as a function of density $\rho$. Error bars are smaller than marks.

**Fig. 8.** Existence probability $E_p$ shown in Fig. 7 is plotted as a function of scaled density $\rho' = (\rho - \rho_c)L^{1/\nu}$.

**Fig. 9.** Configuration of bi-disperse continuum percolation model at critical density is shown.

**Fig. 10.** Estimated values of existence probability $E_p$ of bi-disperse continuum percolation are plotted. The system sizes are $L = 64, 80$ and $128$.

**Fig. 11.** Existence probability of bi-disperse system given in Fig. 10 is plotted as a function of scaled density, $\rho' = (\rho - \rho_c)L^{1/\nu}$. 
differences change only parameter B, do not change the form of existence probability. That is the reason why the finite-size scaling function has the universality.

We also find that the form of $E_p$ depends on boundary conditions and shape of the system, so we can scale $E_p$ only if two systems have the same boundary condition. But, even if boundary conditions are changed, we confirm $\alpha$, the ratio of proportional constant of scaling variables, has universality.

To derive this theory for general percolation model, we only use two assumptions; The correlation function’s form is written as exponential function and to ignore the multi-point correlation. The coincidence of simulation results and derived equation means these assumptions are valid. So this theory is expected to be universal, we can also apply it for other models, such as the Ising model.

We assume the simple exponential behaviour in eq. (2.2), but it is not essential for the argument written in this paper. The assumption works well for simulations we confirmed, but we can choose any other functions for other systems, or for more accurate discussions.

The continuum percolation with size dispersity is studied. We found mono- and bi-disperse systems have the same finite-size scaling function. It means that size dispersity of the soft-core system does not change the form of $E_p$, change only the parameter $B$ like as the difference of types of percolation. Note that we take soft-disk model in this article. In soft-core system, there are no interaction between particles, so it is possible that we cannot see the effect of the size dispersity.

According to Ito, polydispersity plays an important role in fluid-solid transitions of hard-core models. Therefore, it is of interest to study the size dispersity for continuum percolation of hard-core particles.

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