Searching for a New Type of Surface Percolation on a 3D lattice

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ABSTRACT

We consider a new surface percolation problem on a 3D simple cubic lattice through numerical simulation. In this problem, randomly occupied surfaces initially form an infinite cluster at $p = 0.21$, where p is the surface occupation probability. This site percolation problem is well-studied. The infinite cluster at this value of p, however, contains many "hole", since surfaces are considered to be connected if they share at least one edge in common. As p increases over that value, these holes are gradually filled with surfaces. We find that, at $p = 0.66$, there is a sharp transition where the infinite cluster contains one sheet with complicated folds. We also numerically evaluate the critical exponents β and ν using finite size scaling method and obtain $\beta = 0.3$ and $\nu = 1.0$. We cannot find this combination of the values in any sets of critical exponents well-known at present. This fact may suggest that our surface percolation problem belongs to a new universality class.

Keywords: Critical Phenomena, Percolation, Numerical Simulation, Stochastic Process, Modeling of Nature

1 INTRODUCTION

Surface percolation problem has been studied from many point of views. This problem can be applicable to various real problems such as cracking of bulk materials, blocking of liquid percolation, formation of membrane, and so on. Thus thorough understanding of the nature of surface percolation is very important.

Here we consider an elementary surface percolation problem in a three-dimensional (3D) simple cubic lattice. In this problem, surfaces are randomly occupied by a given probability. Two surfaces are referred to be "connected" if they share one edge in common. As increasing the surface occupation probability, p, from zero, the size of the maximum connected surface cluster becomes larger. At $p = 0.21$, an infinite size of cluster emerges for the first time. This percolation problem is well-studied and the nature of the transition is well described by the usual 3D critical exponents.

Let us re-examine this old problem from another point of view. In the ordinary definition of the connectivity, two surfaces are connected if they have one edge in common. In other words, this definition is locally defined. A cluster made up from connected surfaces by this connectivity generally contains many holes. The existence of holes can have important effects in applications to some real problems. For example, if we interpret the occupied surfaces as membranes which prevent a liquid from going through a bulk material, the existence of holes means incomplete blocking of liquid percolation. We thus consider another type of connectivity, which is "globally" defined.

If we increase the surface occupation probability over the percolation threshold, $p = 0.21$, holes in the infinite cluster are gradually filled with surfaces and disappear. We expect that at some value of p the disappearance of the holes reaches some extent such that the infinite cluster contains at least one sheet of connected surfaces with no holes. The conductivity condition that the infinite cluster must have at least one sheet with no holes has a global nature, since the condition of "no holes" cannot be determined unless we investigate the infinite cluster as a whole and related to the topology of the cluster. It is possible that this global connectivity changes the nature of the transition from that defined by local connectivity. It seems, however, that this type of percolation transition defined by global connectivity is not well studied at present. Thus in this paper we approach to this problem through numerical simulations.

This paper is organized as follows. In Section 2, the detail of numerical calculation is described. The results of the calculation are also shown in this section. There we can see that a sharp transition really does exist in this problem. In Section 3, the critical exponents are evaluated using finite size scaling method. Neither the 2D exponents nor the 3D exponents cannot give a good fit. Discussion and the conclusion from our results are found in Section 4.

2 NUMERICAL CALCULATION

2.1 Model

Our model is very simple. Surfaces in a 3D simple cubic lattice are randomly occupied by the probability, p. The connectivity of these surfaces is initially examined locally, that is, two surfaces are connected if they have one edge in common. (See Fig.1.) We choose by this local connectivity the largest cluster from all cluster.. In ordinary percolation problem, connected surface percolation occurs when the size of the largest cluster reaches that of system size. Since our attention is focused on the holeless sheet percolation embedded in this largest cluster, we further investigate the surface cluster.

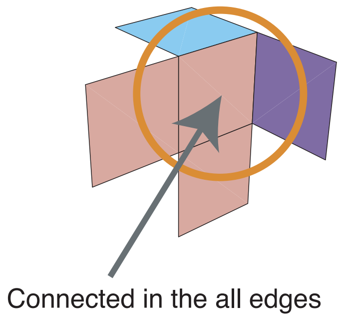

Figure 1: a connected surface in all edges

If the largest cluster contains holes, we can find inner surfaces that have at least one edge which is not connected to any surfaces. We refer to them as "dangling surfaces".

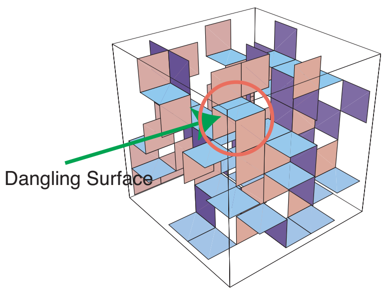

Figure 2: a dangling surface in a locally connected surface cluster

When we find dangling surfaces, we eliminate them. This operation is repeatedly performed and finally we can obtain a holeless backbone embedded in the largest cluster. (See Fig.3.) If this backbone sheet spans the whole system length, we say that holeless sheet percolation occurs.

2.2 Results

We perform numerical simulations of this sheet percolation problem on 3D simple cubic lattices of various system sizes. The system sizes are $L = 4, 8, 12, 16, 20$. At each system size, the ratio of the number of surfaces belonging to the holeless backbone in the largest cluster to the whole surface number, P, is averaged over 100 samples. We also calculate the ratio of the number of

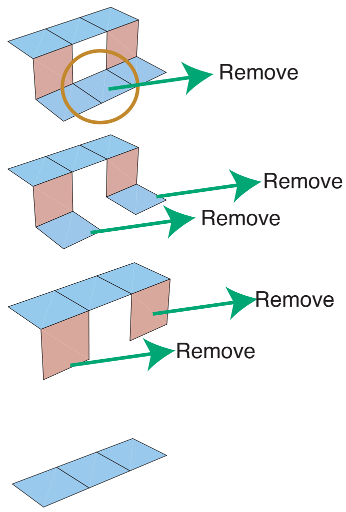

Figure 3: Repeatedly removing dangling surfaces

surfaces belonging to the largest cluster to the number of whole surfaces as a check. These data must show an ordinary percolation transition. The results are shown Fig.4. In this plot, we can clearly see that the sheet percolation occurs t at $p_{c2} \approx 0.66$ after the ordinary percolation at $p_{c1} = 0.21$.

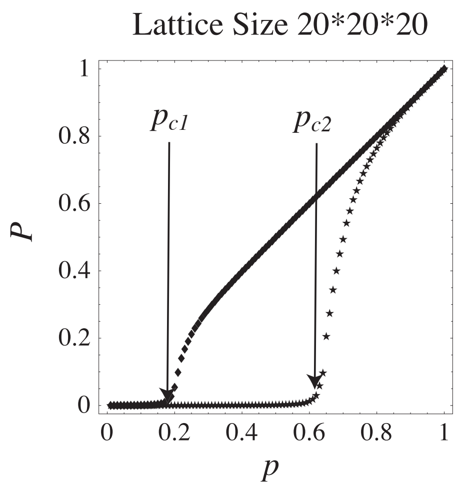

Figure 4: The ratio of the number of surfaces belonging to the holeless backbone to the whole surface number, P, is plotted with respect to the surface occupation probability, p. After the ordinary percolation at p_{c1}, the sheet percolation occurs at $p_{c2} \approx 0.66$.

3 ANALYSIS

In this section, we evaluate the critical exponents, β and ν, of this transition using finite size scaling method.

The exponent β is related to the intensity of the order parameter P as

$$P \sim (p - p_{c2})^{\beta} \quad (p > p_{c2}), \tag{1}$$

and the exponent ν is related to the correlation length ξ as

$$\xi \sim |p - p_{c2}|^{-\nu} \quad (p \approx p_{c2}). \tag{2}$$

In the present calculation, the intensity of the order parameter, P, depends on the system size L as well as the occupation probability p. From the finite size scaling theory[1], various values of P at given values of p and L can be fitted by a single scaling function $F(x)$ as

$$P \cdot L^{\beta/\nu} = F\left((p - p_{c2})\, L^{1/\nu}\right). \tag{3}$$

Data collapsing strongly depends on the values of β and ν. The dependence on the value of p_{c2} is rather weak. It is well known that the values of critical exponents such as β and ν are universal over various transitions if they occur in the same dimensionality. The values for 3D transition are

$$\beta_{3D} = 0.4, \;\; \nu_{3D} = 0.9, \tag{4}$$

and the values for 2D transition are

$$\beta_{2D} = \frac{5}{36} \approx 0.139, \;\; \nu_{2D} = \frac{4}{3} \approx 1.33. \tag{5}$$

Since the sheet transition occurs on a 3D lattice, it is logical to expect that the 3D exponents give the best fit.

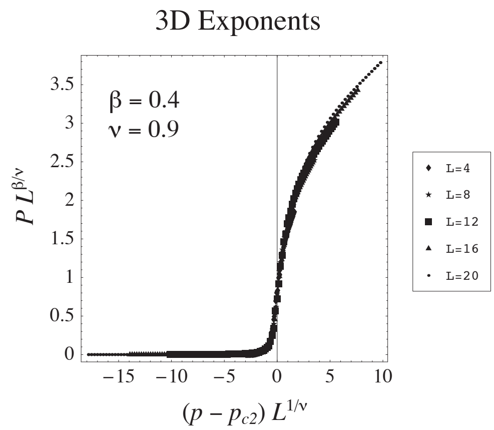

Figure 5: Fitting with the 3D exponents. The percolation threshold p_{c2} is taken to be 0.65 for a good fit.

3.1 Fitting with 3D exponents

Figure 5 shows the fitting with the 3D values of exponents. Though the fitting seems to be good around p_{c2}, it is preferable if we can find values that give a better fit over wider range of $p - p_{c2}$, since the critical region of this transition is expected to be rather wide for these small values of L. We will show at below that the better values of exponents really do exist.

3.2 Fitting with 2D exponents

Figure 6 shows the fitting with the 2D values of exponents. As is expected, the data collapsing is not good, since, clearly, the transition dimensionality is not two..

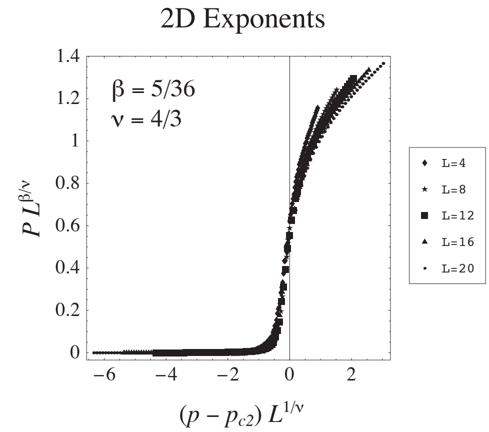

Figure 6: Fitting with the 2D exponents. The percolation threshold p_{c2} is taken to be 0.68 for a good fit.

3.3 Fitting with new exponents

In Fig.7, we show the best fitting we believe at present. The collapsing of data is almost perfect over wider range of $p - p_{c2}$ than the fitting using 3D values of exponents. (See Fig.5.)

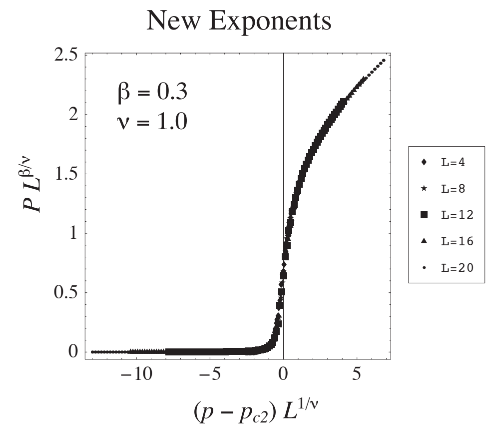

Figure 7: The best fit using new values of exponents. The wide range of data collapsing is striking.We choose $p_{c2} = 0.66$ for the fitting.

4 DISCUSSION AND CONCLUSION

In this numerical calculation, we obtain the values

$$\beta = 0.3, \;\; \nu = 1.0. \tag{6}$$

We cannot find this set of values in the well known chart of critical exponents. Since theoretical reasoning of these deviations from 3D values is lacking, here, we only give a qualitative argument.

The 3D values are

$$\beta_{3D} = 0.4, \ \ \nu_{3D} = 0.9, \tag{7}$$

and the 2D values are

$$\beta_{2D} = \frac{5}{36} = 0.139, \ \ \nu_{2D} = \frac{4}{3} = 1.33. \tag{8}$$

Obtained values (6) are interpreted as that the 3D values are slightly modified and deviate to the direction of 2D values.

Because of the following two reasons, we believe that these deviations are not fictitious but real ones.

- The existence of holes changes the topology of a bulk material. It seems to be quite possible that this topological nature affects the dimensionality of the transition.
- In this percolation problem, the ordinary percolation due to local connectivity initially occurs. After that, the holeless backbone is formed on this loosely connected infinite cluster. It is well known that the infinite cluster made by locally connected surfaces has fractal dimension, even if the transition occurs in integral dimensionality. In other words, the sheet transition occurs on a fractal dimensional lattice. From this consideration, it seems to be natural that the dimensionality of the sheet transition is different from ordinary ones.

We admit that we need more supporting facts for the confirmation of our results. Numerical calculations on larger system sizes must be performed. A through theoretical argument is also needed. These are left for the future study.

In conclusion, a new type of surface percolation problem defined by the connectivity related to global character of surface clusters is studied. The holeless sheet percolates through the infinite connected surface cluster at $p = 0.66$, where p is the surface occupation probability. The critical exponents, β and ν are evaluated using finite size scaling method. These values are $\beta = 0.3$ and $\nu = 1.0$ and fall between the 3D and 2D values. It suggests that this transition occurs on a lattice of fractal dimensionality

REFERENCES

[1] D. Stauffer, "Introduction to Percolation Theory", Taylor & Francis (London and Philadelphia), 1985.