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solution to the problem no. 12
presented by the team of Ukraine

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Powder conductivity

Measure and explain the conductivity of a mixture of metallic and dielectric powders with various proportions of the two components.

Abstract

The proposed problem is considered within the Percolation Theory framework. It is shown that the correct statement of the problem is the determination of the dependence of probability of existence of the conductive path on the number fraction of conductive particles. The upper estimation both for the bond and site percolation threshold for D-dimensional cubic lattice is obtained from combinatorics of "directed" paths. The comparison of theoretical results with experimental data is given. The finite size effects are discussed.

Thanks

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Overview

- General remarks and experimental results
- Theoretical model

1 General remarks and experimental results

The problem proposed refers us to the study of very interesting percolation phenomenon. The scientific activity in this area started from pioneering works of Broadbent S. R. and Hammersley J. M. in 1954–1957. Up to now the problem of running current through dielectric medium (or fluid flow in porous medium) with stochastically distributed conductive regions remains far from its solution.

The statement of general percolation problem for proposed "powder" version of this phenomenon is as following. The system is a powder mixture, which consists of metallic and dielectric grits. Electric current runs through system if metallic particles form a chain that goes from one plate to another. This chain is called the the conductive cluster (CC). When the concentration of metallic particles is small, the probability of formation of CC is extremely small because almost all configurations do not allow the existence of such a long conductive path from one plate to another. When the concentration of conductive grits is large then this path is always present. There could be also other conductive paths. It is obvious that the conductivity of the system equals to conductivity of the contact layer on the surfaces of metallic particles. This value has no significance (at least for the consideration of percolation phenomenon). Therefore one can expect the following qualitative dependence of conductivity σ on the number fraction of conductive elements on concentration of conductive particles p shown schematically on figure 1.

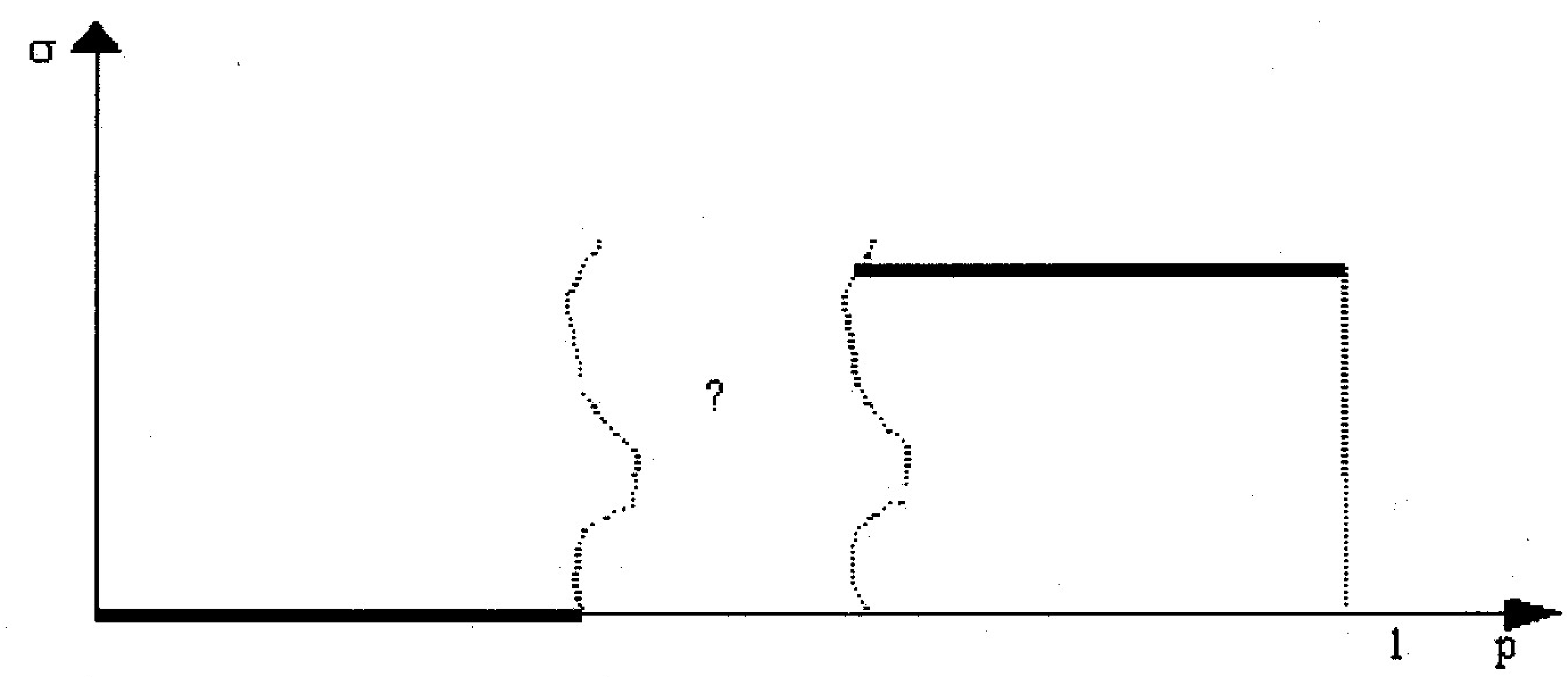

Figure 1: Concentration

Very small fractions correspond to zero probability of CC-existence. The intermediate values of p corresponds to non-zero but less than 1 probability of CC-existence. It means that under such values only definite part of configurations supports the CC-existence. In this case we can not measure the conductivity since it depends on the configuration. It means that the correct statement of the percolation problem is the determination the probability $P(p)$ of existence of CC as a function of p. From physical arguments it is obvious that $P(p)$ is monotone non decreasing function of p. Hence there exists:

$$p^* = \sup\{p : P(p) = 0\} \tag{1}$$

This value is called the percolation threshold (PT). So the expected dependence can be plotted in one of the following way:

The case shown on figure 2 is realized in 2-dimensional case. The possibility of jump discontinuity at p^* for $D > 2$ has not been ruled out that is why figure 2 describes possible behavior. Note that this is according to theoretical background.

We start our consideration from experimental determination of PT. In our experiments we modeled powder system as a mixture of steel and dielectric balls. The container (see figure 4) with electric contact on opposite sides was filled with these balls in different proportions.

To generate random configuration distribution this box was shaken and we checked whether current ran or not. The experiment was repeated 100 times for every proportion to get the statistics. As a results of these experiments we obtained the following graph, presented on figure 5:

It shows the dependence of probability of appearance of CC on p – the concentration of metallic particles in powder mixture. We can see that maximum of the derivative $\frac{\partial P}{\partial p}$ that indicates the

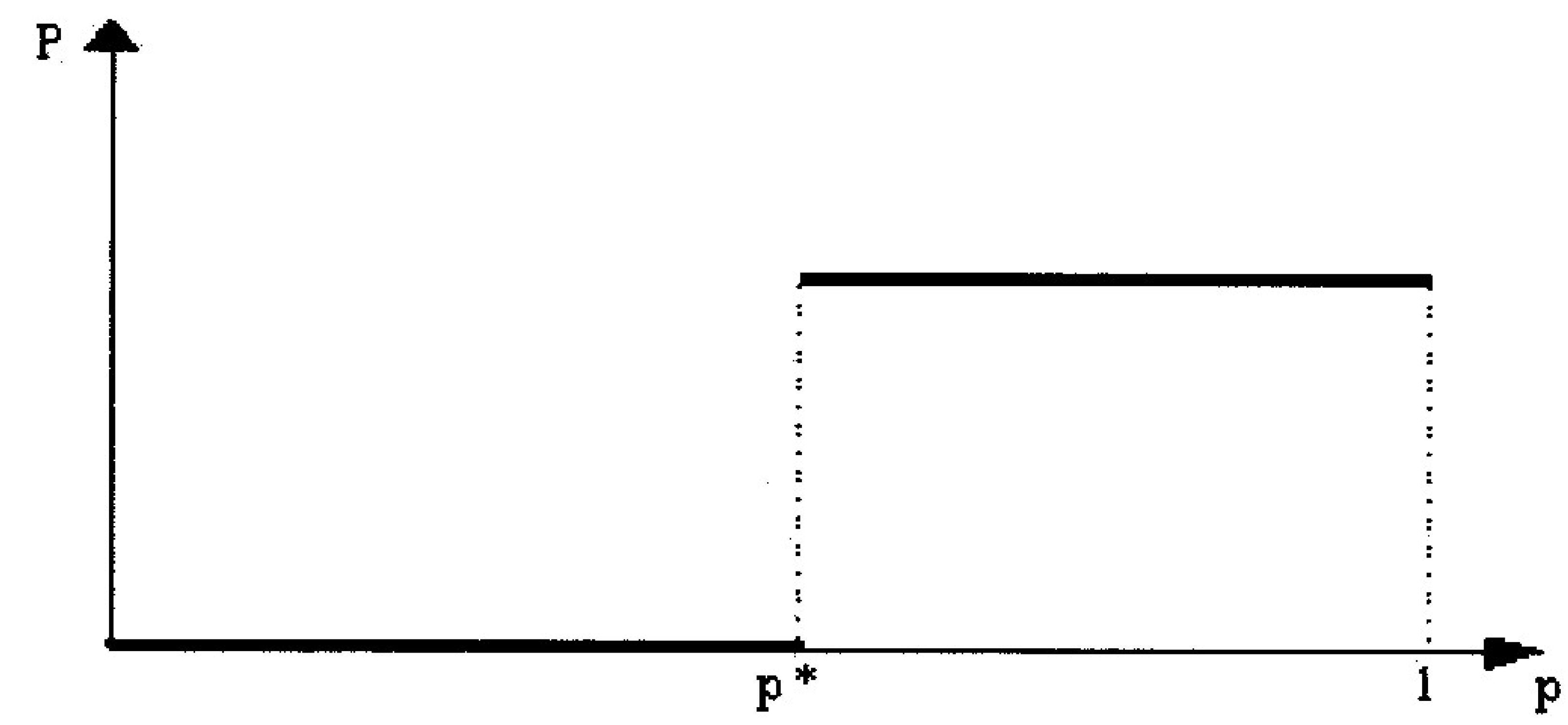

Figure 2: PT – 2-dimensional

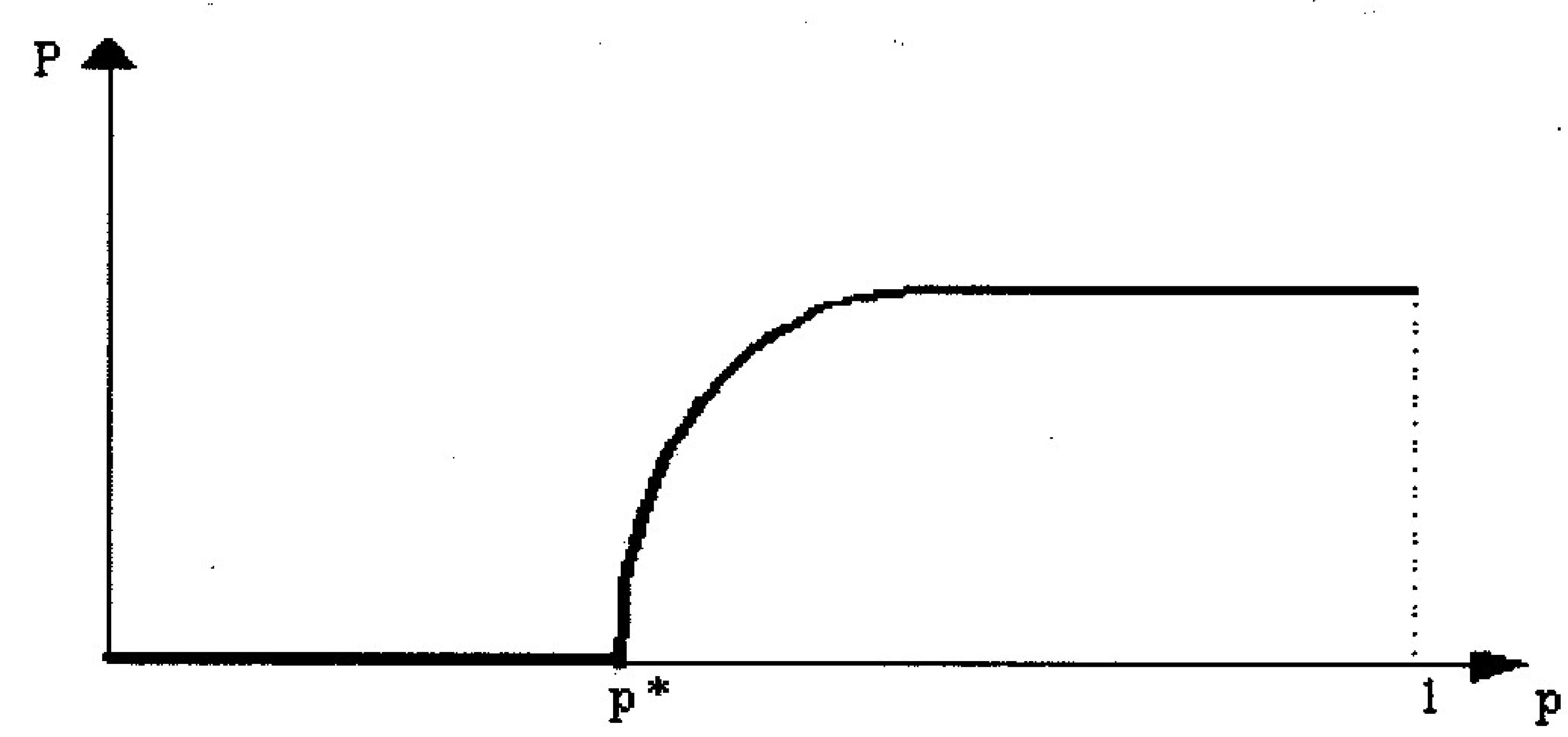

Figure 3: PT – 3-dimensional

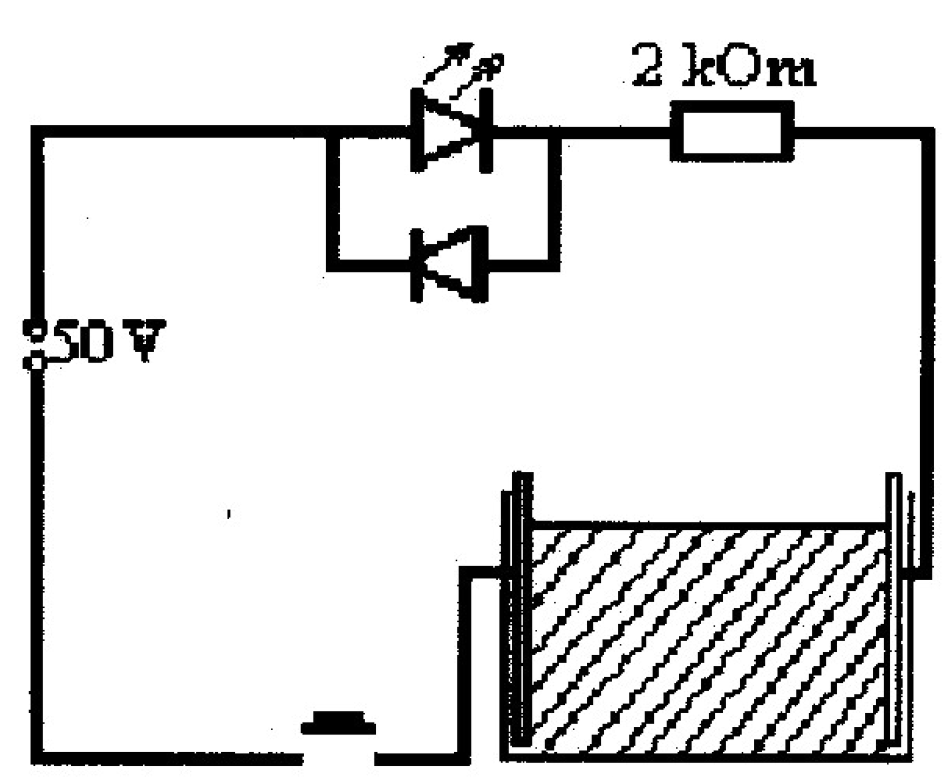

Figure 4: Set-up

threshold value of $p(p^*)$ is near $p^* = 0.35$.

2 Theoretical model

Now let us consider the problem of determining the value of p^* theoretically. Strictly speaking this consideration refers to site percolation problem in 3 dimensions. In rigorous mathematical sense the PT is defined only for infinite system. Otherwise, when the concentration is $\frac{r}{L}$ there is the only configuration when the array goes from one side to another. Here r is the radius of a ball, L the length of the system. It is obvious that the probability of occurrence of such a configuration in even distribution tends to zero if $L \to \infty$. So we come to statement of site percolation problem for random packing of the spheres. The rigorous solution of this problem remains open in spite of many approaches and techniques applied. Here we try to make a simple upper estimation for the PT basing on simple combinatorial consideration. At first we consider simpler problem of bond percolation on cubic lattice.

Just for the sake of simplicity we consider the square lattice $m \times n$. Let us find the average number of conductive paths from low site of left hand corner side with coordinates $(0,0)$ to upper right hand corner $(m > 0, n > 0)$. Among all paths connecting these points there are the paths which can be one-to-one projected on the diagonal of the rectangular $(0,0)$; $(m,0)$; $(0,n)$; (m,n). They

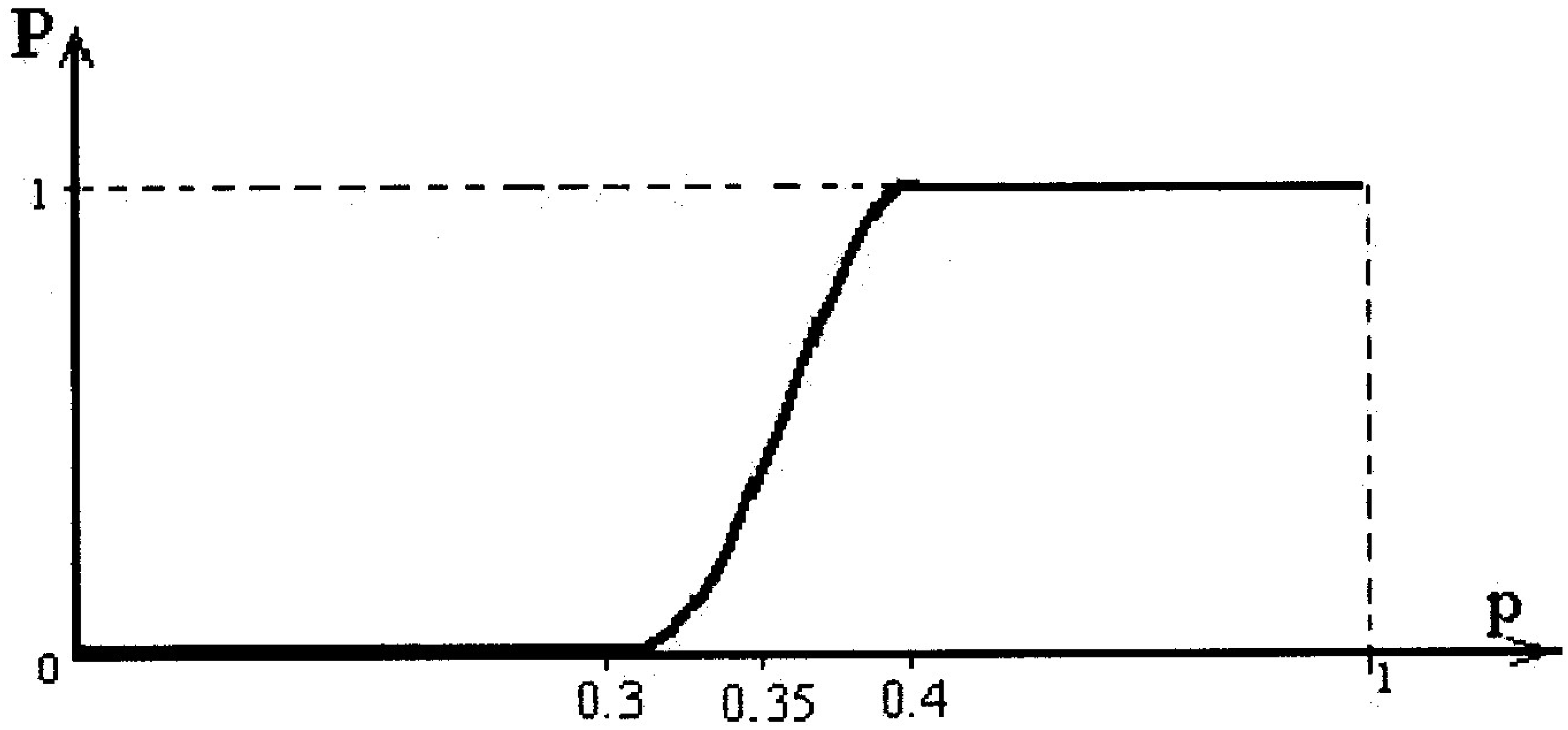

Figure 5: Experimental data

consist on $m+n$ bonds and we call them as directed. It is easy to calculate the number of directed paths:

$$N_{\text{dir}} = \frac{(m+n)!}{m!n!} \tag{2}$$

The probability of a given path to be conductive is

$$P_{\text{cond}} = q^{m+n} \tag{3}$$

where q is the concentration of conductive bonds. Therefore the average number of directed conducted paths is:

$$N_{\text{cond}} > N_{\text{dir}} P_{\text{cond}} = \frac{(m+n)!}{m!n!} q^{m+n} \tag{4}$$

Using STIRLING asymptotic for factorial

$$n! = \sqrt{2\pi} e^{-n} n^{n-\frac{1}{2}} \left(1 + o(1)\right) \tag{5}$$

we get

$$\begin{aligned} N_{\text{cond}} \quad > \quad & \left(\left(n+m-\frac{1}{2} \right) \ln(m+n) - \left(m - \frac{1}{2} \right) \ln(n) \right. \\ & \left. - \left(m - \frac{1}{2} \right) \ln(m) + (m+n) \ln(q) - \frac{1}{2} \ln(2\pi) \right) \left(1 + o(1)\right) \end{aligned} \tag{6}$$

To find the PT we need consider the limit $m, n \to \infty$ which corresponds to infinite lattice. Let us define the parameter

$$k = \frac{m}{n}$$

which corresponds to certain direction to infinity. Obviously, PT can be determined as:

$$q^* = \max_{0<k<1} q(k) \quad \text{where} \quad q(k) = \sup_{0<q<1} \{ q : \lim_{n\to\infty} N_{\text{cond}}(q) = 0 \} \tag{7}$$

This condition means that if $q < q^*$ there is not any path (in average) going to infinity. From (6) and (7) it is easy to get:

$$q(k) \leq \frac{k^{\frac{k}{k+1}}}{1+k} q^* < \frac{1}{2} \tag{8}$$

This result together with other arguments gives $q^* = 0.5$ for square lattice. It is the shortest way to get this famous result of Percolation Theory. For cubic 3-D lattice in analogous way we get:

$$N = \frac{(n_1 + n_2 + n_3)!}{n_1! n_2! n_3!} \tag{9}$$

$$\sup q(x,y) = \frac{e^{\frac{x \ln x + y \ln y}{1+x+y}}}{1+x+y} \tag{10}$$

$$x = \frac{n_2}{n_1} \tag{11}$$

$$y = \frac{n_3}{n_1} \tag{12}$$

$$q^* \leq \frac{1}{3} \tag{13}$$

Known numerical results give the estimation $q^* \approx 0.25$. Similarly in general case of D-dimensional cubic lattice one can get in analogous way

$$q^* \leq \frac{1}{D} \tag{14}$$

There exists also lower estimation for q^*. It reads:

$$q^* \geq \frac{1}{2D-1} \tag{15}$$

It is easy to see that the combinatorial approach proposed is also valid for site percolation problem. Little change should be made in (3) since $m+n$ bond corresponds to $m+n+1$ sites and q is interpreted as the conductive site fraction. But the estimation (14) remains unchanged:

$$q^* < p^* \leq \frac{1}{D} \tag{16}$$

Comparison this estimation with numerical results $p^* \approx 0.31$ shows very good agreement with obtained experimental value of $p^* = 0.35$ (see figure 5). Note that the last value is greater then other two ones. This fact is naturally explained as following. The packing of the grits in a box was less dense than cubic packing. Hence the PT for such packing should be greater than PT for more densely packed structure. Note that combinatorial approach proposed can be applied to other regular lattices.