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d-dimensional conductivity, conductivity exponent, and critical concentration in the site problem

M. A. Soliman
Department of Physics, Faculty of Science, Mansoura University, Mansoura, Egypt

E. Ahmed
Department of Mathematics, Faculty of Science, Mansoura University, Mansoura, Egypt
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We generalize grey scaling to d dimensions and calculate the electrical conductivity of a hypercubic network. The critical exponent t and the site percolation threshold p_c are estimated for $2 \leq d \leq 6$. The values obtained are in good agreement with those obtained theoretically or by other methods.

I. INTRODUCTION

Studying the electrical properties of a percolating random resistor is an important problem in the subject of critical phenomena of inhomogeneous materials. They have been investigated both theoretically[1-5] and experimentally.[6,7] All theoretical studies of the electrical conductivity, apart from Ref. 5, have solved Kirchoff's equations at each site. This is not always an easy task and is time consuming.

In a previous paper[5] the method of grey scaling has been introduced in two and three dimensions. It is significantly simpler than solving Kirchoff's equations. Moreover, it can even be implemented using small personal computers. Furthermore, it gives acceptable values for the critical concentration p_c, the conductivity S, and the conductivity exponent t given by

$$S \sim (p-p_c)^t \quad (p > p_c) , \tag{1}$$

despite use of a small lattice.

In this paper we generalize grey scaling to a general d dimension. We then calculate p_c, S, and t in four, five, and six dimensions using computer simulation.

We did not proceed for higher d since it is known[8] that $d=6$ is the critical dimension for percolation theory and our results are in excellent agreement with the expected value from mean-field theory. We will compare it to the previously proposed formulas.[9,10]

II. GREY SCALING IN GENERAL DIMENSIONS

Scaling[9] is one of the most useful ideas in condensed matter and field theory. In ordinary scaling [say in a two-dimensional (2D) random resistor network] a square lattice is replaced by a single supersite. This supersite is considered conducting if the current can pass across the original lattice, otherwise the supersite is considered an insulator. This idea is successfully used to calculate p_c and the critical exponents ν and t.

Grey scaling is a hybrid of computer simulation and a real-space renormalization group. As an illustration we apply it to a two-dimensional square lattice, shown in Fig. 1. This is renormalized into a supersite with conductivity C given by

$$C = \frac{1}{1/C_1 + 1/C_2} + \frac{1}{1/C_3 + 1/C_4} , \tag{2}$$

where C_1, C_2, C_3, and C_4 are the conductivities of the sites. The resulting super cells are renormalized and so on until we get the bulk conductivity. Therefore in grey scaling we do not solve Kirchoff's equations at each site. This is a great advantage since solving these equations is by no means an easy task and we invite the reader to look at Straley's comments[3] about them. Moreover, the simplicity of grey scaling has enabled us to use only personal computers to study the random site problem. The cell renormalization in Fig. 1 has been used before[11] in a theoretical study of the site-diluted resistor networks. The real-space renormalization group has been applied there to get p_c and t in two dimensions. There is no repetition between this paper and ours since grey scaling is a simulation method. Using it we are able to calculate C, p_c, and t for all dimensions $2 \leq d \leq 6$, as shown later on. From the theoretical point of view grey scaling is a real-space renormalization. This is a well-established method and ensures the correctness of grey scaling. The limitations of grey scaling are those of real-space renormalization which has been studied before.[12]

The transformation in 2D is

$$p' = p^4 + 4p^3(1-p) + 2p^2(1-p)^2 , \tag{3}$$

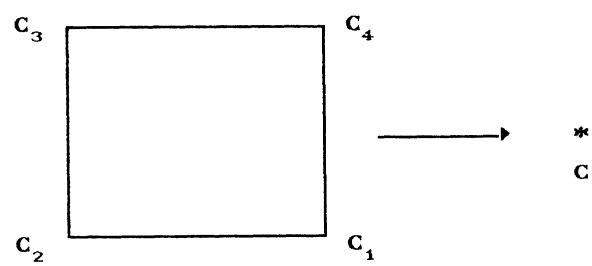

FIG. 1. Schematic illustration of the transformation process of four sites in a square lattice to a supersite with conductivity C.

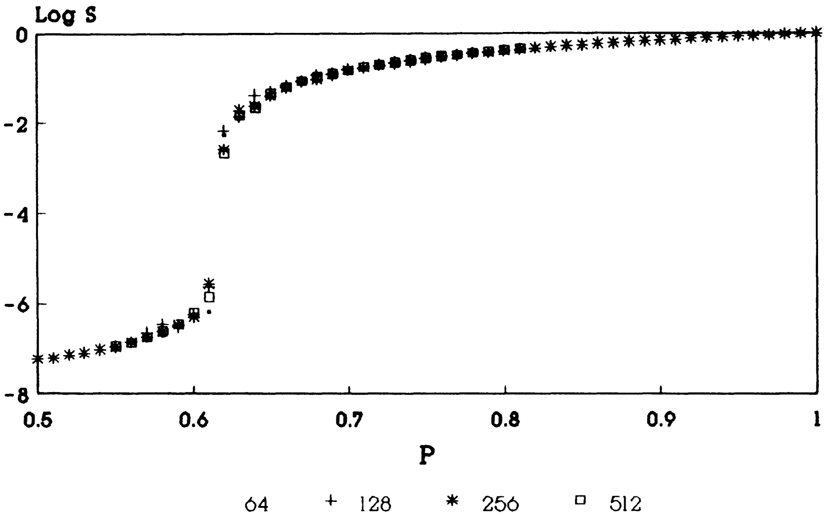

FIG. 2. The conductivity in 2D for different lattice sizes.

which gives $p_c = 0.618$ for $d = 2$. We will see that this is in excellent agreement with the value obtained in our simulation (0.6183). The grey scaling transformations for $3 \leq d \leq 6$ are listed in the Appendix. In Fig. 2 the conductivity is shown in 2D for different lattice sizes ranging from 64 to 512. The figure clearly shows that the method improves as the lattice increases as well as giving good results for small lattices. This ensures that this method is correct at least in two dimensions.

We generalize grey scaling to calculate p_c, t, and S in any dimension. To do this let us imagine a hypercube in d dimensions whose sites have conductivities $S(I_1, I_2, \ldots, I_d)$ where $I_1, I_2, \ldots, I_d$ are the coordinates of the site. Without loss of generality we take the direction of the potential difference to be along the first axis. We sum the resistances which are in a series. They are determined as follows: There are d terms $\mathcal{K}_i$, $i = 1, 2, \ldots, d$ given by

$$\mathcal{K}_a = R(I_1, I_2, \ldots, I_a + 1, \ldots, I_d) + R(I_1 + 1, I_2, \ldots, I_a + 1, \ldots, I_d)\,, \tag{4}$$

$$a = 2, 3, \ldots, d\,,$$

$$\mathcal{K}_1 = R(I_1, I_2, \ldots, I_d) + R(I_1 + 1, I_2, \ldots, I_d)\,, \tag{5}$$

Then there are $\binom{d-1}{2}$ terms $\mathcal{K}_{kl}$ where $d \geq l > k \geq 2$ given by

$$\mathcal{K}_{kl} = R(I_1, I_2, \ldots, I_{k-1}, I_k + 1, I_{k+1}, \ldots, I_l + 1, \ldots, I_d) + R(I_1 + 1, I_2, \ldots, I_k + 1, \ldots, I_l + 1, \ldots, I_d)\,. \tag{6}$$

There are $\binom{d-1}{3}$ terms $\mathcal{K}_{klm}$, $d \geq m > l > k \geq 2$ defined by

$$\mathcal{K}_{klm} = R(I_1, I_2, \ldots, I_k + 1, \ldots, I_l + 1, \ldots, I_m + 1, \ldots, I_d) + R(I_1 + 1, I_2, \ldots, I_k + 1, \ldots, I_l + 1, \ldots, I_m + 1, \ldots, I_d)\,, \tag{7}$$

and so on until we reach the final term $\mathcal{K}_{k_1 k_2 \cdots k_{d-1}}$ given by

$$\mathcal{K}_{k_1 k_2 \cdots k_{d-1}} = R(I_1, I_2 + 1, I_3 + 1, \ldots, I_d + 1) + R(I_1 + 1, I_2 + 1, I_3 + 1, \ldots, I_d + 1)\,, \tag{8}$$

The total number of these resistances is 2^{d-1}. Then the conductivity $\mathcal{C}(I_1, I_2, \ldots, I_d)$ of the equivalent supersite is

$$\mathcal{C}(I_1, I_2, \ldots, I_d) = \sum_{i=1}^{d} 1/\mathcal{K}_i + \sum_{l > k = 2}^{d} 1/\mathcal{K}_{kl} + \cdots + 1/\mathcal{K}_{k_1 k_2 \cdots k_{d-1}}\,. \tag{9}$$

The argument for the validity of grey scaling is the same as ordinary scaling, namely systems near phase transition are scale invariant,[13] consequently they are self-

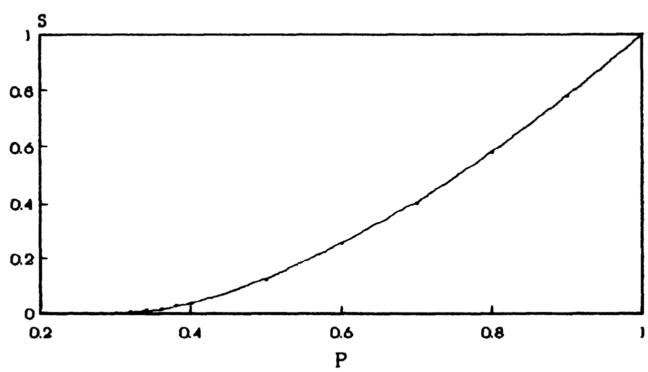

FIG. 3. Dependence of the conductivity S on the concentration of the conducting phase p for $d = 3$.

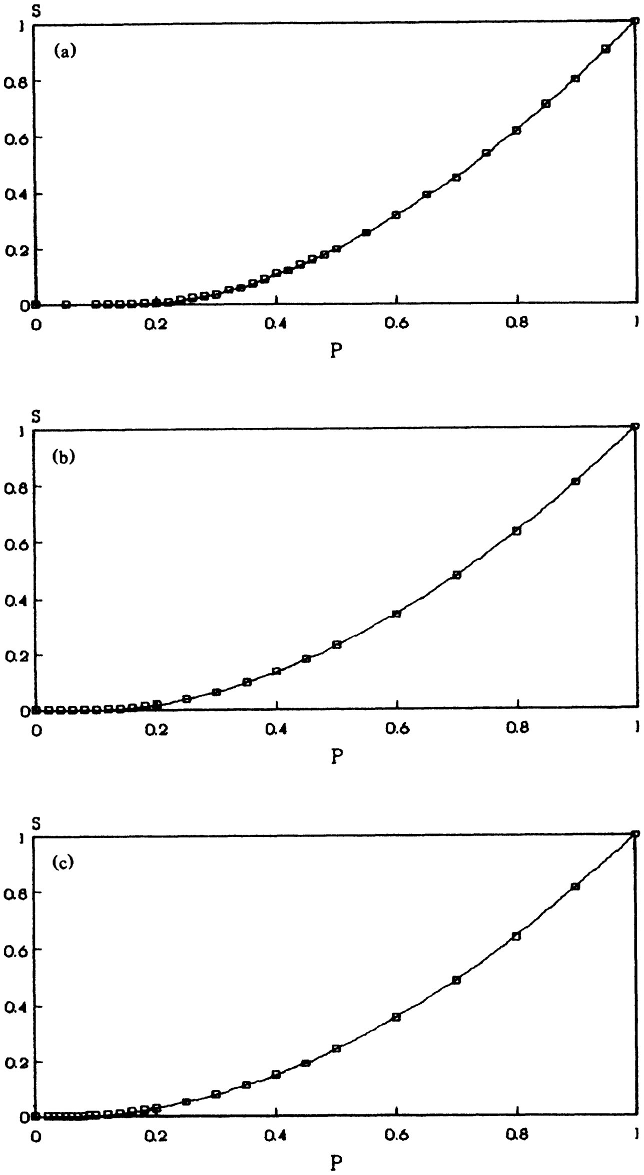

FIG. 4. The same as Fig. 3 for (a) $d=4$, (b) $d=5$, and (c) $d=6$.

similar. Therefore, lumping several small units should reproduce the original system. Hence after a sufficient number of scalings we will obtain a super, super, ... supersite which is equivalent to the original network.

From a practical point of view the simplicity, efficiency of grey scaling, and the ability to use it on microcomputers makes it, in our opinion, better than the usual simulation methods to calculate p_c, t, and C.

III. RESULTS AND DISCUSSION

A binary system consisting of two phases of conductances, 1 and 10^{-8}, was studied from two to six dimensions. Figure 3 shows the conductivity S as a function of the concentration of the conducting phase p for a three-

TABLE I. Values for p_c and t in dimensions $d=2$–6.

d	p_c	t
2	0.6183	1.2711
3	0.2845	1.7446
4	0.1384	2.4167
5	0.0728	2.7522
6	0.0306	3.0000

dimensional system.

Both p_c and t are calculated from the previous figures, and the following values for p_c and t were obtained:

$$t=1.2711\pm0.004,\quad p_c=0.6183\pm0.002\,,\quad \text{for } d=2\,,$$

$$t=1.7446\pm0.003\,,\quad p_c=0.2845\pm0.002\,,\quad \text{for } d=3\,.$$

These values agree with the presently accepted values.[9]

We generalize grey scaling by four, five, and six dimensions and our results are shown in Fig. 4. The obtained values for t and p_c are given in Table I. In Table II we compare our results for t with other choices offered in the literature.[9,10] The obtained value for t at $d=6$ is in excellent agreement with the theoretically expected value ($=3$). This gives further credibility to our method. Our results for p_c are valid only for $2\le d\le 6$ since p_c changes with d without saturation.

Grey scaling has been applied to determine the conductivity, the critical concentration, and the conductivity exponent for a site-diluted network for all dimensions $d\le 6$. The results obtained for $d=2$, $d=3$, and $d=6$ agree with those obtained by other methods. It has both the advantages of real-space renormalization and the advantage of simulation methods. It has more advantages than real-space renormalization, e.g., calculation of conductivity and studying $d>2$ problems without much difficulty. Also, it has more advantages than the usual simulation methods[1-3] since we do not need to solve Kirchoff's equations at each site and we do not have problems with convergence. To get a feeling of what this means we recall that ordinary simulation methods require that Kirchoff's equations are solved at each of the 2^d sites of the unit hypercubic cell, $2^d=4$, 8, 16, 32, and 64 for $d=2$, 3, 4, 5, and 6, respectively.

We conclude that grey scaling is a new and quite useful simulation method.

APPENDIX

The grey scaling transformations in dimensions $3\le d\le 6$.

In this appendix we list the scaling transformations for $3\le d\le 6$. We have listed the transformation for $d=2$ in Eq. (3). For $d=5$ and 6 the transformations are very long, therefore, for these dimensions, we list only the dominant terms, i.e., those with contributions $\ge 10^{-3}$.

For $d=3$:

TABLE II. Comparison of the present results for t with values from Refs. 9 and 10.

	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	
t_1	1.14	1.35	1.64	1.83	$\cdots$	$t_1=1+\beta$
t_2	1.33	1.66	2.04	2.16	$\cdots$	$t_2=(d-1)\nu$
t_3	1	1.83	2.36	2.62	$\cdots$	$t_3=1+(d-2)\nu$
t_4	1.28	1.70	2.28	2.67	$\cdots$	$t_4=1+2\beta$
t_5	1.33	1.86	2.38	2.56	$\cdots$	$t_5=(5d-6)\nu/4$
t_6	1.26	1.90	2.40	2.55	$\cdots$	$t_6=[(3d-4)\nu-\beta]/2$
t_s	1.27	1.74	2.42	2.75	3.00	t_s — our

$$1-p'=(1-p)^8+8p(1-p)^7+24p^2(1-p)^6+32p^3(1-p)^5+16p^4(1-p)^4 . \tag{A1}$$

For $d=4$:

$$1-p'=(1-p)^{16}+16p(1-p)^{15}+112p^2(1-p)^{14}+448p^3(1-p)^{13}+1120p^4(1-p)^{12}+1792p^5(1-p)^{11} +1792p^6(1-p)^{10}+1024p^7(1-p)^9+256p^8(1-p)^8 . \tag{A2}$$

For $d=5$:

$$1-p'\cong(1-p)^{32}+32p(1-p)^{31}+480p^2(1-p)^{30}4480p^3(1-p)^{29}+29\,120p^4(1-p)^{28}+153\,216p^5(1-p)^{27} +512\,512p^6(1-p)^{26}+146\,432p^7(1-p)^{25}+5\,706\,220p^8(1-p)^{24}+5\,857\,280p^9(1-p)^{23}+\cdots . \tag{A3}$$

For $d=6$:

$$1-p'\cong(1-p)^{64}+64p(1-p)^{63}+1984p^2(1-p)^{62}+39\,680p^3(1-p)^{61}+575\,360p^4(1-p)^{60}+892\,800p^5(1-p)^{59} +59\,794\,287p^6(1-p)^{58}+(4.3083\times10^8)p^7(1-p)^{57}+\cdots . \tag{A4}$$

[1] S. Kirckpatrick, Rev. Mod. Phys. **45**, 574 (1973).
[2] I. Webman, J. Jorter, and M. Cohen, Phys. Rev. B **11**, 2885 (1975).
[3] J. P. Straley, Phys. Rev. B **12**, 5722 (1977).
[4] J. Zabolisky and D. Stauffer, J. Phys. A **19**, 3705 (1986).
[5] E. Ahmed, A. Tawansi, and M. A. Soliman, Phys. Lett. A (to be published).
[6] B. Watson and P. Leath, Phys Rev. B **11**, 4893 (1974).
[7] T. Noh, S. Lee, Y. Song, and J. Gaines, Phys. Lett. **114A**, 207 (1986).
[8] M. Stephen, Phys. Rev. B **15**, 5674 (1977).
[9] D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1985).
[10] S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).
[11] J. Yeomans and R. Stinchcombe, J. Phys. C **11**, 4095 (1978).
[12] A. Young and R. Stinchcombe, J. Phys. C **8**, L535 (1975).
[13] A. Belavin, A. Polyakov, and A. Zamoldchikov, Nucl. Phys. **B241**, 333 (1984).