A new method for the calculation of the conductivity of inhomogeneous systems

2005 J. Phys. A: Math. Gen. 38 5057

(http://iopscience.iop.org/0305-4470/38/23/001)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 5057–5067 doi:10.1088/0305-4470/38/23/001

A new method for the calculation of the conductivity of inhomogeneous systems

M S Byshkin and A A Turkin

National Science Center Kharkov Institute of Physics and Technology, Akademicheskaya str. 1, 61108 Kharkov, Ukraine

E-mail: byshkin@kipt.kharkov.ua and anatole.turkin@kipt.kharkov.ua

Received 18 January 2005, in final form 7 April 2005
Published 25 May 2005
Online at stacks.iop.org/JPhysA/38/5057

Abstract

A new method for computing the conductivity of random irregular resistor networks is developed. This method is a generalization of the transfer-matrix technique, proposed by Derrida and Vannimenus for regular 2D and 3D lattices. At the same time for large systems the method presented in this paper is more efficient than the transfer-matrix technique. To demonstrate the method it is applied to a cubic lattice at the percolation threshold and away from it. The conductivity has been found for lattices with size up to 324^3. The ratio between the conductivity exponent t and the correlation length exponent η was estimated to be $t/\eta = 2.315$, in good agreement with the literature data.

PACS numbers: 02.70.+c, 05.50.+q

1. Introduction

A broad range of problems in physics of materials involves disordered media, whose effective behaviour is dominated by connectedness of its particular component. Examples are porous media, sea ice, doped semiconductors, etc. The effective conductivity of an inhomogeneous medium is one of the central problems of the modern theory of transport phenomena in disordered systems [1, 2]. Here conductivity is understood in the wide sense—it may be mass or heat transfer as well as other macroscopic transport properties, the determination of which is similar to the solution of a problem of electroconductivity of an inhomogeneous medium. The numerical solution of such a problem can be formally reduced to the solution of a set of Kirchhoff equations [2]. Finding the solution of this set of equations meets well-known computational difficulties. Various numerical methods were developed to overcome them. The Kirchhoff equations can be solved by iterative methods [3, 4], by special network transformations [5, 6] and by techniques of the transfer-matrix [7, 8]. It was established that the conductivity σ of a random mixture of conducting and nonconducting elements behaves

as $\sigma \propto (p - p_c)^t$, when $p \to p_c$ where p is the fraction of conducting elements, p_c is the percolation threshold and t is the conductivity exponent.

In spite of a large number of papers devoted to the calculation of the conductivity exponent, its exact value is still unknown even for the most investigated 3D lattices. The absence of efficient methods for the calculation of the conductivity of large networks of resistors remains the main obstacle for the calculation of the conductivity exponent.

In this paper the new exact method for the calculation of the conductivity of random irregular networks of resistors is proposed. It is similar to the method of transfer-matrix [7], but it has the following advantages: (i) it can be used for calculation of the conductivity of inhomogeneous systems, and (ii) its numerical implementation is high speed. The method is efficient for large networks and is convenient for calculation of the conductivity away from the percolation threshold. The estimation of the method's speed and efficiency is presented in section 3.

To demonstrate the method the conductivity of a cubic lattice is calculated for $p \geqslant p_c$. The results are presented in section 4. For $p = p_c$ the conductivity is calculated for lattices of sizes from 9^3 to 324^3. It is shown that for network sizes larger than 64^3 the boundary conditions affect the conductivity of the network weakly. The results for the conductivity of lattices ranging in size from 64^3 to 324^3 were used to estimate t/η, where η is the correlation length exponent. The conductivity of the lattice was also calculated for $p > p_c$ for lattice sizes up to 180^3. These results were used to estimate the value of the conductivity exponent t directly, which was found to be in good agreement with estimates of other authors.

2. Description of the method

The method we propose can be used to calculate the conductivity of an arbitrary resistor network with the following natural restrictions: (i) on a macroscopic scale the sites of a network are to be distributed uniformly, and (ii) resistors should not connect very distant sites of a network.

In contrast to the transfer-matrix method [7], where sites are added to the investigated part of network one by one, in our method sites are added by blocks of sites. This makes the method a little bit more complicated, but increases its efficiency and significantly reduces the restrictions on networks that can be studied. The method can be used for systems of any dimension, both for lattices and irregular networks. For simplicity we describe the method using a 2D square lattice.

To calculate the relative conductivity, the conductance of a $L \times L$ square lattice is calculated. The sites of the first and the Lth columns are connected by zero resistance conductors and form two sites, the resistance between which is to be calculated. The periodic boundary conditions are imposed in the perpendicular direction. The entire network is divided into blocks (figure 1).

The restrictions mentioned above mean that each block consists of about the same number of sites, and two sites are connected with a resistor if they are either in the same or in neighbouring blocks.

The resistor network is investigated by parts, block by block, till the entire network is analysed. In figure 1 the blocks are numbered according to the order of their investigation. The result of a block investigation is the transfer-matrix, elements of which are conductances between external sites of block (see section 2.1). As discussed in section 2.2, blocks are investigated one after another and are appended to the part of the network already investigated; thereby we obtain the transfer-matrix for the entire investigated part of the network. The final

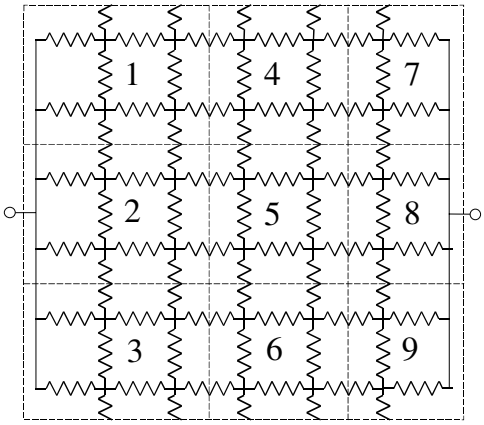

Figure 1. Division of the network into blocks.

result of the network investigation is the 2×2 transfer-matrix, the absolute value of its elements is equal to the required network conductance.

As the block size decreases the method degenerates into the transfer-matrix method [7]. If the whole network is investigated as one block, then the method corresponds to the direct solution of the system of Kirchhoff equations. In principle, such calculations are also possible but they require considerable computer resources [3].

2.1. Definitions

The sites are neighbours if they are connected by a resistor. Consider the set B of network sites. We denote sites of the set B which have neighbours outside B as external sites of B. Single out the subset $E \subset B$ of external sites and denote the remaining sites belonging to $B \,|\, E$ as internal (figure 2(*a*)).

Let U be the column vector of potentials of sites of set B,

$$U = \begin{pmatrix} W \\ V \end{pmatrix}$$

where V and W are the column vectors of potentials of internal and external sites of set B correspondingly.

Denote the sum of currents from all sites $i' \in B$ to site $i \in B$ as I_i, the sum of currents from all site $i' \in B$ to site $i \in E$ and $j \in B \,|\, E$ as I_i^W and I_j^V correspondingly. In the matrix form

$$I = \begin{pmatrix} I^W \\ I^V \end{pmatrix}.$$

We need to find the matrix D that satisfies the relation

$$I^W = DW. \tag{1}$$

By analogy with [7] we will call D the transfer-matrix for the set of sites B.

The I_i^W may be written in the following form:

$$I_i^W = \sum_{j \neq i} \frac{W_i - W_j}{r_{ij}} = W_i \sum_{j \neq i} \frac{1}{r_{ij}} - \sum_{j \neq i} \frac{1}{r_{ij}} W_j, \tag{2}$$

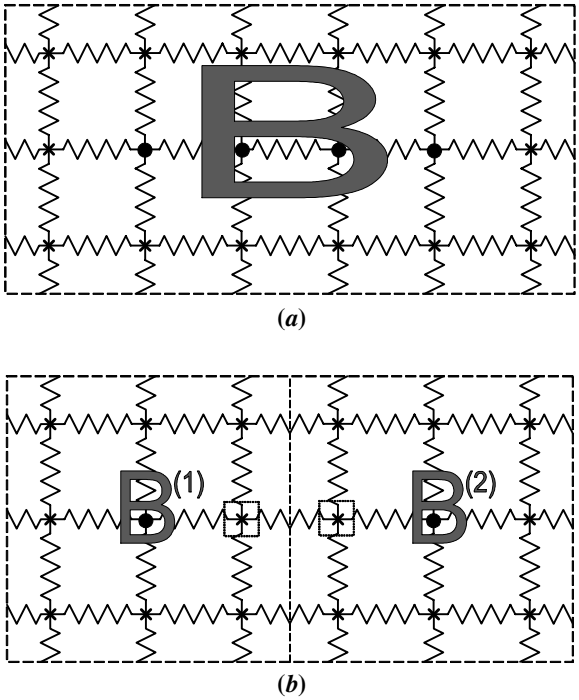

Figure 2. Schematic illustration of joining two blocks. Circles are internal sites, crosses are external sites. (*a*) The union of blocks $B^{(1)}$ and $B^{(2)}$; (*b*) Blocks $B^{(1)}$ and $B^{(2)}$. The squares are sites from sets $E^{(1)}|E$ and $E^{(2)}|E$.

where r_{ij} is the resistance of the network between two external sites i and j. Comparing (1) and (2) we find that the elements of the transfer-matrix satisfy the following conditions:

$$(1) \quad D_{ij} = D_{ji} = -\frac{1}{r_{ij}} \qquad \text{for} \quad i \neq j,$$

$$(2) \quad D_{ii} = \sum_{j \neq i} \frac{1}{r_{ij}} \qquad \text{or} \qquad \sum_{j} D_{ij} = 0.$$

Thus to find the network conductance between two external sites it is enough to construct the transfer-matrix for the set of sites of this network.

2.2. Construction of transfer-matrix

The sum of currents I_i may be written in the following form:

$$I_i = \sum_{i' \in B} \frac{U_i - U_{i'}}{R_{ii'}},$$

where summation is over all neighbours of site i, $R_{ii'}$ is the resistance of the resistor connecting sites i and i'. In the matrix form

$$I = TU, \tag{3}$$

off-diagonal and diagonal elements of matrix T are given by correspondingly

$$T_{ij} = \begin{cases} -\dfrac{1}{R_{ij}}, & i \quad \text{and} \quad j \text{ are neighbours} \\ 0, & i \quad \text{and} \quad j \text{ are not neighbours} \end{cases}$$

$$T_{ii} = -\sum_{j \neq i} T_{ij}.$$

The matrix T may be partitioned as follows

$$\begin{pmatrix} I^W \\ I^V \end{pmatrix} = \begin{pmatrix} T^{(2)} T^{(1)} \\ T^{(1)^T} T^{(3)} \end{pmatrix} \begin{pmatrix} W \\ V \end{pmatrix}. \tag{4}$$

According to the Kirchhoff law $I^V = 0$. Then from (1) and (4) we find the transfer-matrix

$$D = T^{(2)} - T^{(1)} T^{(3)^{-1}} T^{(1)^T}. \tag{5}$$

Now the block structure can be substantially simplified. Indeed, as soon as the transfer-matrix of the block is known, the resistors and the internal sites of this block can be replaced by the resistors between external sites i and j with resistance $-1/D_{ij}$.

In order to construct the transfer-matrix for the whole network we need a procedure for finding the transfer-matrix for the union of two neighbouring blocks (sets of sites) with known transfer-matrices. Consider two nonoverlapping sets of sites $B^{(1)}$ and $B^{(2)}$ which are neighbours (i.e., some sites from $B^{(1)}$ are neighbours of sites from $B^{(2)}$ (figure 2(b)). Construction of transfer-matrices for these sets is equivalent to elimination of their internal sites. However, the union of the simplified blocks still contains internal sites, which are neighbouring external sites of sets $B^{(1)}$ and $B^{(2)}$. The structure of this union is further simplified by elimination of its internal sites, i.e. by construction of its transfer-matrix

Using the algorithm described here, one can construct the transfer-matrix for the whole network.

3. Estimation of the algorithm speed

Suppose the algorithm is not in the initial stage or the final one. As soon as periodic boundary conditions are imposed, the number of external sites M' of the investigated part of the network does not change considerably when a new block is added to it. To estimate the number of operations that the algorithm requires it is enough to estimate the number of operations connected with the addition of a new block to the investigated part of network, that is the number of operations required by equation (5) to find the transfer-matrix for (i) a new block, and (ii) its union with the investigated network.

From the theory of numerical methods [9] it is known that (i) the number of operations required to find an inverse matrix for $N \times N$ matrix is proportional to N^3, and (ii) the number of operations to multiply matrix $L \times N$ by matrix $N \times M$ is proportional to LNM. Denote the approximate ratio of these numbers of operations by a. Denote the number of sites in a new block as N and the number of its external sites as M. Neglecting the number of operations required to sum up two matrices, the number of operations required to find the transfer matrix for the new block is proportional to $(N - M)^3 + aNM(N - M)$. The number of sites considered to unite this new block with the investigated network equals $M + M'$, the number of external sites of the union is M', hence the number of operations required by (5) to find the transfer-matrix for the union of the new block with the investigated network is proportional to

$$M^3 + aMM'(M + M').$$

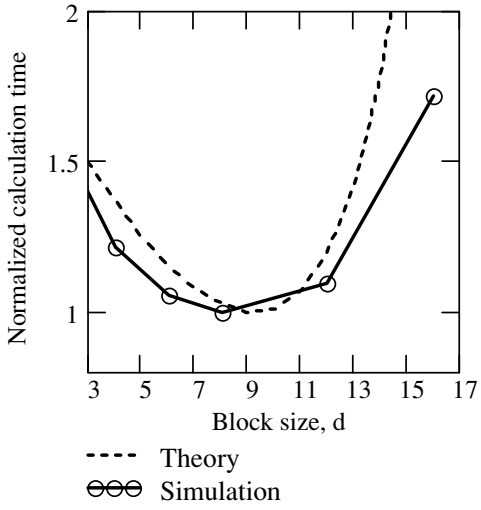

Figure 3. The relative calculation time as a function of block size d for a cubic lattice of size $L \times L \times L = 48 \times 48 \times 48$. The calculation time is normalized to the minimum calculation time for the corresponding curve.

The ratio of the number of operations for finding the transfer-matrix for the whole network to the number of sites in this network is about the same as the ratio of the number of operations for adding a new block to the number of sites in this block, and is proportional to

$$t(N, M, M') = \frac{(N-M)^3 + aNM(N-M) + M^3 + aMM'(M+M')}{N}. \quad (6)$$

Hence the method requires $t(N, M, M')n$ operations, where n is the number of sites in the whole network.

It turns out that an optimum block size exists which minimizes the number of operations required by the algorithm, that is $t(N, M, M')$ can be minimized. To show this, here we consider a cubic lattice of size $L \times L \times L$ with periodic boundary conditions in two directions, all bonds of which have resistance equal to 1. Note that the resistance of this lattice is known *a priori* and is equal to $1/L$; we are interested in the simulation time only.

N, M and M' are functions of the network size L and the block size d. For the cubic lattice $M' \approx L^2$, $M = d^3 - (d-2)^3$, $N = d^3$. The relative calculation time t versus block size d is shown in figure 3. Both the results of numerical calculations and the dependence given by (6) are presented for the lattice size $L = 48$. According to figure 3 the optimum size of the block exists, which minimizes $t(N(d), M(d), M'(L))$. For a 450 MHz processor the minimum calculation time equal to 230 min is reached at $d = 8$. For comparison the time to calculate the conductance of this lattice at the percolation threshold is several seconds only.

By numerical minimization of (6) for different L, we have found that for $L > 32$ the optimum block size scales with L as $d_{\min} \propto L^b$. Then for large L the minimum calculation time $t \propto L^c$ (at $d = d_{\min}$). For a varying in a rather wide range from 0.1 to 1 the exponent $b = 0.56 \pm 0.01$ and the exponent $c = 3.46 \pm 0.01$. Hence for large 3D systems the proposed method requires $tn = tL^3 \approx L^{6.46}$ operations. For comparison the transfer-matrix technique [7] requires L^7 operations. If we used $d \ll L$, we would have $t(N, M, M') \propto M'^2 \approx L^4$ and the number of operations for our method would also scale as L^7. For a 2D lattice the transfer-matrix technique [7] requires L^4 operations, and the number of operations of our method scales as $L^{3.6}$. Similar to the transfer-matrix technique [7], our method is extremely

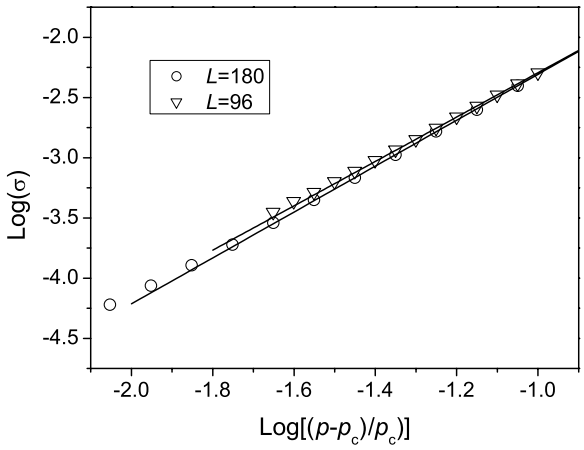

Figure 4. The conductivity of the lattice near the percolation threshold. Solid lines determine the slope of the curves and are used to estimate the conductivity exponent.

efficient for random bands, i.e. for resistor networks of size $L \times L \times H$. In this case our method requires $L^{5.46}H$ operations and it is O(N) method.

4. Application of the method for the cubic lattice

In this section the method described above is used for the calculation of the relative conductivity σ of a cubic lattice of size $L \times L \times L$ with the bond conductance equal to 1 with the probability p and 0 with the probability $1 - p$.

The matrix inversions are used in the method. They are not singular if the network is connected. To obtain its connectedness, the network was replaced with its percolation cluster. Since the conductivity is usually calculated near the percolation threshold, the extraction of the percolation cluster decreases the number of network sites significantly [2]. The number of sites was further decreased by extraction of the percolation skeleton, i.e. by cutting off the dangle branches of the percolation cluster. To extract the percolation cluster and the cluster skeleton the recursive algorithms were used, the number of operations of which is proportional to the number of sites in the percolation cluster. Therefore, the transformations of the network which use recursive procedures require much less computation time than the procedure for calculation of the conductance. After the transformations of the network, we applied our method. It takes only several seconds to calculate the conductance of the cubic lattice of size 260^3 on a computer based on a Pentium 450 MHz processor, similar to the computer used in [6]. At the same time the method described in [6] required about 5 min. The limitation for the largest possible size of lattice L is determined by the amount of computer memory.

The result of computations was the 2×2 matrix. It was proved in section 2.1 that the absolute values of its elements must be the same. Of course they were a little bit different because of intrinsic computational errors, but this difference was small. The relative conductivity was calculated by normalizing the conductance by the lattice size. Below we analyse the properties of the relative conductivity.

As p decreases the conductivity decreases too. For large systems it tends to zero as $\sigma \propto (p - p_c)^t$ when $p \to p_c$. To determine the conductivity exponent t the conductivity was calculated for p values near the percolation threshold p_c. The dependence $\sigma(p)$ is shown in figure 4 for lattices of sizes $L = 180$ and $L = 96$. The value of $(p - p_c)/p_c$ varies in the

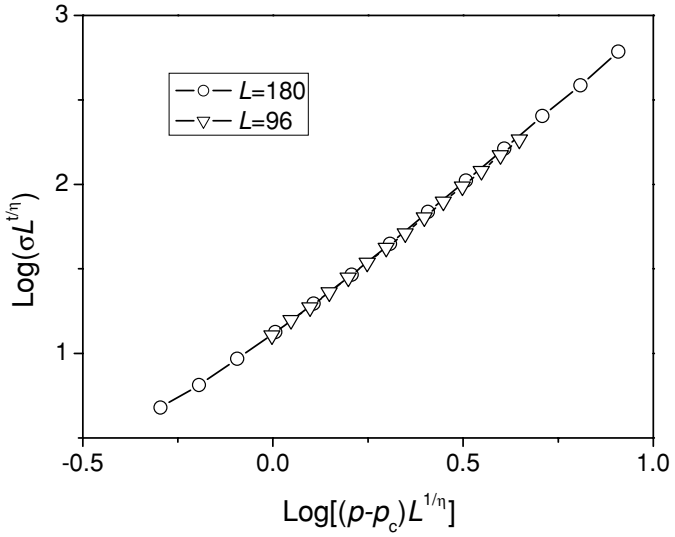

Figure 5. Verification of correspondence of the computational results to the scaling relation (7) for lattices of sizes $L = 96$ and $L = 180$.

interval from 0.005 to 0.1. The number of realizations was 120 to 500 depending on p. For these values of L and p the percolation cluster was always present.

Because of finiteness of the network, the conductivity is not zero even when $p = p_c$, i.e. for p values very close to p_c the power law $(p - p_c)^t$ is violated. The slope α of curves in figure 4 gives the estimation of the conductivity exponent t. It depends on size L. For $L = 96$, $\alpha \approx 1.84$, and for $L = 180$, $\alpha \approx 1.90$. It is clear that with increasing L the value of α will grow and tend to the value of conductivity exponent t. In [10] the upper limit for the conductivity exponent is suggested to be $t \leqslant 2$.

Together with direct calculations of the exponent t the finite-size scaling is often used in the literature [2, 11, 12]. Near the percolation threshold the conductivity depends on the size of the system L as $\sigma = L^{-t/\eta} f_1(L/\xi)$. Here ξ is the percolation correlation length, which scales as $\xi \propto (p - p_c)^{-\eta}$ when $p \to p_c$ and η is the correlation length exponent (for the 3D cubic lattice $\eta \approx 0.88$ [2]). For the systems with $L \geqslant \xi$, the following scaling relation can be written as

$$\sigma = L^{-t/\eta} f(L^{1/\eta}(p - p_c)), \tag{7}$$

and for $L \ll \xi$

$$\sigma(L) = AL^{-t/\eta}. \tag{8}$$

To check the scaling relation (7) the results of calculations presented in figure 4 were replotted in the form of the function $f(L^{1/\eta}(p - p_c)) = \sigma L^{t/\eta}$ (figure 5). We used the following values $\eta \approx 0.88$ [2] and $t/\eta \approx 2.3$ [3, 6]. One can see that sets of data for different L follow the same curve, which proves the existence of scaling (7).

For $p = p_c$ we have $L \ll \xi$ and the conductivity can be written in the form given by (8), which is often used to estimate the ratio t/η [3–8]. If the value of η is known, such an estimation allows one to find the conductivity exponent t by computing conductivity of relatively small systems. We calculated the conductivity for networks of sizes $L = 9$, 14, 18, 28, 42, 64, 96, 144, 260, 324 at $p = p_c$. The number of realizations was 15 627, 10 046,

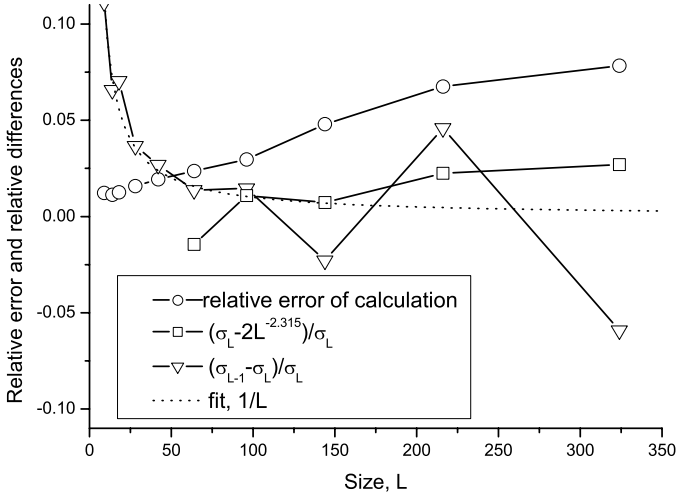

Figure 6. The relative error of computations (circles), $(\sigma_L - 2L^{-2.315})/\sigma_L$ (boxes) and $(\sigma_{L-1} - \sigma_L)/\sigma_L$ (triangles) versus the lattice size. The dotted line is the function $1/L$, which is a good fit for $(\sigma_{L-1} - \sigma_L)/\sigma_L$.

7813, 5023, 3348, 2197, 1465, 976, 703, 540 and 430 accordingly. The value of p_c for the cubic lattice is known with good accuracy $p_c = 0.248\,8126 \pm 5 \times 10^{-7}$ [13]. The obtained data are in good agreement with (8). The relative error of calculations of $\sigma(L)$ is shown in figure 6 as a function of L. The value $2D/\sqrt{N}$ was chosen as the error of calculation, where D is the standard deviation and N is the number of realizations.

To obtain a good estimate for the value of t/η one has to be careful with the boundary conditions in the system under study, otherwise the surface effects will interfere with the effects of finite-size scaling [5, 14]. Recently the energy dissipation methods were proposed for calculating the network conductivity [3, 6]. In these methods the influence of boundary conditions is less strong than in the method proposed here. However, the influence of boundary conditions was not investigated in [3, 6]. It is only clear that this influence diminishes with increasing size of the system. To investigate the influence of boundary conditions we calculated the conductivity σ_L and σ_{L-1} of the networks of sizes $L \times L \times L$ and $L \times L \times (L-1)$, correspondingly. The relative difference $(\sigma_{L-1} - \sigma_L)/\sigma_L$ is shown in figure 6 as a function of L. One can see that the relative difference of the conductivities of these lattices is less than the relative error of our calculations for $L > 64$. As could be expected, the boundary conditions have strong influence on the conductivity of the network only when the size of this network is small, i.e. $L < 64$. Fitting the results for the conductivity σ_L of networks in the size interval from 64 to 324 with equation (8) we obtain $\sigma \approx 2L^{-2.315}$, $t/\eta = 2.315$. The obtained estimate is in good agreement with recent data, $t/\eta = 2.282$ [3] and $t/\eta = 2.305$ [6]. Note that the largest size of the network used in our calculation is more than twice as large as that used in [6] and about four times larger than that used in [3]. Using the value $\eta \approx 0.88$ one finds $t \approx 2.0$. This estimation of the conductivity exponent is only 5% different from the estimation of the conductivity exponent we have obtained without using finite-size scaling for the lattice of size $L = 180$.

We used a simple form of finite-size scaling (see (7) and (8)). Recently Janssen and Stenull [15] have made a careful analysis of corrections to finite-size scaling. Figure 5 shows that corrections to (7) are not very significant for the sizes used. We did not use the corrections

to (8) because for all the sizes L used to estimate t/η the absolute value of the difference $\sigma_L - 2L^{-2.315}$ was less than the statistical error of our calculation (figure 6).

In our calculations we used the value of the percolation threshold obtained in [13], which appears to be the most accurate to date. For example, the estimates of Grassberger 0.248 814 $\pm$ 3 $\times$ 10^{-7} [16] and Tomita and Okabe 0.248 81(3) [17] are less accurate. We checked if our estimate of the exponent t/η is sensitive to possible inaccuracy in the value of percolation threshold p_c used. A new series of calculations was made for this purpose. Using in our calculations a value of p_c different from that used before by 10^{-5} (0.004%) we have obtained a value of t/η changed by about 0.02 (0.94%). Thus, the estimate of t/η strongly depends on the accuracy of the p_c value. The value of conductivity exponent t, which was obtained without using finite-size scaling, shifted by less than 0.002 (0.1%), i.e. it is one order of magnitude less sensitive to this shift of the percolation threshold.

5. Conclusions

The detailed description of the numerical method for calculation of the transport phenomena in inhomogeneous media is presented. The described method is the generalization of the well-known transfer-matrix method [7] to the case of irregular networks. The division of the network into blocks which are investigated separately makes this method more efficient and reduces the restrictions on the network topology significantly. The method can be applied to any inhomogeneous media in any dimension, but it is most efficient for 2D and 3D systems.

The estimation of the efficiency of the method was carried out. It was determined that an optimum block size exists which minimizes the calculation time. This method enables one to compute the conductivity of 2D and 3D systems of sizes that were not reached earlier by commonly used relaxation methods. In contrast with relaxation methods our method gives the conductivity of the network exactly.

The method described in this paper was applied to the cubic lattice. It was found to be efficient for calculation of the conductivity of the network both at the percolation threshold and away from it. The conductivity exponent value obtained without using the finite-size scaling technique was only 5% different from that obtained by means of finite-size scaling. This feature of the method enables one to estimate the conductivity exponent for systems that were not investigated earlier, for which the correlation length exponent is unknown and finite-size scaling cannot be applied.

Acknowledgments

The authors are grateful to Dr N P Lazarev for useful discussions and to Professor A S Bakai for the support of this work.

References

[1] Bergman D J and Stroud D 1992 *Solid State Phys.* **46** 14
[2] Stauffer D and Aharony A 1994 *An Introduction to Percolation Theory* 2nd edn (London: Taylor and Francis)
[3] Batrouni G G, Hansen A and Larson B 1996 *Phys. Rev.* E **53** 2292
[4] Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574
[5] Gingold D B and Lobb C J 1990 *Phys. Rev.* B **42** 8220
[6] Clerc J P, Podolskiy V A and Sarychev A K 2000 *Eur. Phys. J.* B **15** 507
[7] Derrida B and Vannimenus J 1982 *J. Phys. A: Math. Gen.* **15** l557
[8] Derrida B, Zabolotski J G, Vannimenus J and Stauffer D 1984 *J. Stat. Phys.* **36** 31
[9] Samarski A A and Gulin A V 1989 *Numerical Methods* (Moscow: Nauka) in Russian

[10] Golden K M 1997 *Phys. Rev. Lett.* **78** 3935
Golden K M, Ackley S F and Lytle V I 1998 *Science* **282** 2238
[11] Cardy J 1981 *Finite-Size Scaling* (Amsterdam: North Holland)
[12] Privman V 1988 *Finite-Size Scaling and Numerical Simulation of Statistical Systems* (Singapore: World Scientific)
[13] Lorenz C D and Ziff R M 1998 *Phys. Rev.* E **57** 230
[14] Hermann H J, Derrida D and Vannimenus J 1984 Rapid communications *Phys. Rev.* B **30** 4080
[15] Janssen H-K and Stenull O 2004 *Phys. Rev.* E **69** 026118
[16] Grassberger P 1992 *J. Phys. A: Math. Gen.* **25** 5867
[17] Tomita Y and Okabe Y 2002 *J. Phys. Soc. Japan* **71** 1570