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Precise determination of the conductivity exponent of 3D percolation using exact numerical renormalization

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Abstract. We present detailed description of a computer method for the calculation of the conductivity of inhomogeneous systems based on an exact renormalization group transformation. We study by this method the effective conductivity of the three-dimensional resistor network at the percolation threshold. For lattices ranging in size from 4^3 to 140^3 we measure the dissipation, finding $t/\nu_{\rm p} = 2.305(15)$, where t is the conductivity exponent and $\nu_{\rm p}$ is the correlation length exponent.

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1 Introduction

Effective conductivity of an inhomogeneous media is one of the central problems of the modern theory of transport phenomena. In the present paper we are interested in the transport properties of the composites or granular or porous materials with a macroscopic scale of inhomogeneity [1-3]. In such a material, there are small, yet much larger than atomic regions where macroscopic homogeneity prevails and where the foregoing macroscopic parameters suffice to characterize the physics. However, different regions may have quite different values for those parameters. If we are interested in physical properties at a scale much larger than those regions and at which the material appears to be homogeneous, then the macroscopic behaviour can again be characterised by bulk effective values, for example, an effective conductivity $\sigma_{\rm e}$. Because both the small scale behaviour (inside the different homogeneous regions) and the overall large-scale behavior are now governed by the same laws of classical physics, the connection between the properties on the two scales is rather strong. Suppose that a material can be characterized by the local electric conductivity $\sigma(\mathbf{r})$ so that the local current density $\mathbf{j}(\mathbf{r})$ and local electric field $\mathbf{E}(\mathbf{r}) = -\nabla \phi(\mathbf{r}) + \mathbf{E}_0$ are connected *via* usual Ohm's law $\mathbf{j}(\mathbf{r}) = \sigma(\mathbf{r}) (-\nabla \phi + \mathbf{E}_0)$, where \mathbf{E}_0 is an external electric field and ϕ is a local potential that fluctuates due to inhomogeneity of the systems. The charge conservation law $\operatorname{div} \mathbf{j}(\mathbf{r}) = 0$ can be written in the following form

$$\nabla \left[\sigma(\mathbf{r})\left(-\nabla \phi\left(\mathbf{r}\right) + \mathbf{E}_{0}\right)\right] = 0.$$
(1)

Solution of equation (1) gives the field and current distribution in the system. Then the effective conductivity $\sigma_{\rm e}$ that characterizes the bulk properties of an inhomogeneous system is defined as

$$\langle \mathbf{j}(\mathbf{r}) \rangle = \sigma_{\mathrm{e}} \mathbf{E}_0,$$
 (2)

where $\langle \dots \rangle$ stands for the volume average. When the composite medium is macroscopically uniform, then the bulk effective conductivity $\sigma_{\rm e}$ is an intensive material parameter – its value is independent of the volume and of the precise nature of the macroscopic boundary conditions, provided those too are macroscopically uniform. Consequently, the particular choice of boundary conditions used to find the fluctuating potential ϕ does not affect the value $\sigma_{\rm e}$ obtained from equations (1, 2). We will use the "natural" boundary condition $\phi(\mathbf{r}) = 0$ at the boundary of the system, from which it follows that the averaged electric field $\langle \mathbf{E}(\mathbf{r}) \rangle$ coincides with the external field $\langle \mathbf{E}(\mathbf{r}) \rangle = (1/V) \int (-\nabla \phi(\mathbf{r}) + \mathbf{E}_0) \, \mathrm{d}V = \mathbf{E}_0$, where V is the volume of the system.

When some of the components are anisotropic, the definitions must be modified appropriately. For other physical properties, such as mass and heat transport, thermoelectric power, magnetotransport and elastic stiffness, a similar discussion can be developed that results in equations analogous to equations (1, 2) to determine the corresponding effective parameters [2].

To use a computer method for solution the partial differential equation (1) it is presented as a set of linear algebraic equations that could be solved numerically. The cubic lattice is usually used for this purpose, but more sophisticated graphs that reflect internal geometry of the system might be considered also (see *e.g.* [4]). In any case

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equation (1), being discretized, reduces to the set of Kirchhoff's equations determined for each site "k" of the graph.

$$\sum_{j} \sigma_{kj} \left(\phi_j - \phi_k + E_{kj} \right) = 0, \qquad (3)$$

where the summation is over the neighbours "j" of the site "k", the potentials ϕ_k and ϕ_j are electric potentials of the site "k" and "j", the conductivities σ_{kj} represent the local conductivity $\sigma(\mathbf{r})$ between site "k" and "j". The electromotive forces (EMF) E_{kj} in equation (3) stand for the external electric field \mathbf{E}_0 applied to the system; $E_{kj} = -E_{jk}$ (see Appendix A).

We present here detailed description of a method for solution of Kirchhoff's equations (3), that we refer as exact numerical renormalization (ENR). The ENR can be used to calculate the potentials ϕ_k and currents

$$j_{kj} = \sigma_{kj} \left(\phi_j - \phi_k + E_{kj} \right) \tag{4}$$

flowing in a graph of any dimension, connectivity, etc. The applied field can be homogeneous or inhomogeneous. Moreover, the proper choice of EMF E_{kj} in equations (3) allows us to simulate systems with intrinsic EMF where electric current may flow even in the absence of the external field. Examples of such systems include composites containing metal grains and solid or liquid electrolytes that form local galvanic elements. Since various problems of transport theory reduce to the continuity equation (1)that in turn is equivalent to Kirchhoff's equations (3), the effective method for the solution of equation (3) is important for the actual calculation of various bulk effective parameters. Careful analysis of Kirchhoff's equations (3) also gives an insight into general features of transport phenomena in composites. The proposed ENR method is most efficient when the underlying graph, where Kirchhoff's equations are determined, has hierarchical structure. It might be, for example, fractal or another geometrical object with low connectivity [1,5]. Note that the most interesting and hard to understand transport phenomena do appear near a critical point where the fluctuations of local parameters have a structure that can be considered in rough approximation as hierarchical (see, e.g., [6,7]). Then the ENR method might be applied validly to find transport coefficients.

In this paper we illustrate the advantages of the ENR method by calculating the effective conductivity of a percolating system. A broad range of problems in the physics of materials involve highly disordered media whose effective behaviour is dominated by the connectedness, or percolation properties, of a particular component. Examples include porous media, doped semiconductors, smart materials such as piezoresistors and thermistors, radar absorbing composites, thin semicontinuous metal films, sea ice, etc. (see [1–5,8–11] and references therein). In modeling transport properties in such materials, a twocomponent random media with component conductivities σ and $\sigma' \ll \sigma$ is often considered. The volume fraction of the components is p and 1-p correspondingly. When conductivity σ' of the "dielectric" component is equal to zero, $\sigma'=0,$ a classical metal-dielectric transition takes place in a percolating system at the concentration p known as the percolation threshold $p_{\rm c}$. The effective conductivity $\sigma_{\rm e}$ decreases with decreasing p and vanishes as $\sigma_{\rm e} \sim (p_{\rm c}-p)^{t/\nu_{\rm p}}$ when the concentration of the conducting component p approaches $p_{\rm c}$ from above, where t is the conductivity exponent and $\nu_{\rm p}$ is the percolation correlation length exponent.

The rest of the paper is organized as follows: In Section 2 we describe our computer method, in Section 3 we consider how the method works for the simplest model-the Sierpinskii Gasket, in Section 4 we calculate conductivity in 3d bond percolating problem and determine the critical exponent $t/\nu_{\rm p}$, Section 5 is devoted to discussion of the results.

2 Exact numerical renormalization (ENR) of Kirchhoff's equations

The problem of the bulk effective conductivity of an homogeneous medium can be approximated by a set of Kirchhoff's equations (3), which are determined on an appropriate chosen graph (see Appendix A). To solve Kirchhoff's equations we express the potential ϕ_k of the site "k" in equation (3) in terms of the potentials ϕ_i of its neighbours.

$$\phi_k = \frac{\sum_j \sigma_{kj} \left(\phi_j - E_{kj}\right)}{\sum_j \sigma_{kj}},\tag{5}$$

where the summation in equation (5) is over neighbours of the site "k". If this expression for the potential ϕ_k is substituted in other of Kirchhoff's equations the site k is eliminated from the system. The potential ϕ_k appears in Kirchhoff's equations for the sites "j" that are neighbouring the site "k". For a particular site "i", which is connected to the site "k", Kirchhoff's equation (3) can be written as

$$\sigma_{ik} \left(\phi_k - \phi_i + E_{ik}\right) + \sum_j \sigma_{ij} \left(\phi_j - \phi_i + E_{ij}\right) + \sum_m \sigma_{im} \left(\phi_m - \phi_i + E_{im}\right) = 0, \quad (6)$$

where the first term is due to the direct connection between sites "k", and "i"; the sum in the second term is over the sites "j" that are simultaneously connected to the sites "k", and "i"; the sum in the last term in equation (6) is over all neighbours "m" of the site "i" that are *not* connected to the eliminated site "k". We substitute in equation (6) the expression (5) for the potential ϕ_k and obtain after simple algebraic transformations the following equation

$$\sum_{j} \sigma_{ij}^{*} \left(\phi_{j} - \phi_{i} + E_{ij}^{*} \right) + \sum_{m} \sigma_{im} \left(\phi_{m} - \phi_{i} + E_{im} \right) = 0$$
(7)

where the first sum goes through the neighbours "j" of the eliminated site "k" while the second sum is still over

all neighbours "m" of the site "i" that are not connected to the eliminated site "k". The new conductivity σ_{ij}^* is given by

$$\sigma_{ij}^* = \sigma_{ij} + \sigma_{ij}',\tag{8}$$

where the conductivity σ'_{ij} is equal to

$$\sigma_{ij}' = \frac{\sigma_{ik}\sigma_{kj}}{\sum_n \sigma_{kn}},\tag{9}$$

where the sum in the denominator is over all neighbours of the decimated site "k". The new EMF E_{ij}^* in equation (7) is equal to

$$E_{ij}^{*} = \frac{\sigma_{ij}}{\sigma_{ij}^{*}} E_{ij} + \frac{\sigma_{ij}'}{\sigma_{ij}^{*}} E_{ij}', \qquad (10)$$

where

$$E'_{ij} = E_{ik} + E_{kj}.$$
 (11)

We can repeat the above procedure for all neighbours "i" of the site "k". That is we replace the potential ϕ_k in Kirchhoff's equations for the sites "i" by formula (5). Then Kirchhoff's equations for the sites "i" take form of equation (7) that does not include the potential ϕ_k . Thus, we eliminate potential ϕ_k from the whole set of Kirchhoff's equations. In other words, we decimate the site "k" from the system.

The decimation of the site "k" results in the renormalization of conductivities and EMFs of the neighbours of the site "k". Suppose that sites "i₁" and "i₂" are neighbours of the site "k". After decimation of the site "k" the conductivity between sites "i₁" and "i₂" changes from initial value $\sigma_{i_1i_2}$ to $\sigma_{i_1i_2}^*$ given by equation (8) and the EMF $E_{i_1i_2}$ changes to $E_{i_1i_2}^*$ given by equation (10). If the neighbours "i₁" and "i₂" of the site "k" have not been connected at all, a new connection between them is established. The new bond conductivity $\sigma_{i_1i_2}^* = \sigma'_{i_1i_2}$ and EMF $E_{i_1i_2}^* = E_{i_1i_2}'$ are given by equations (9, 11) respectively. Since the ENR transformation is exact it does not change the solution of Kirchhoff's equations. That is, all potentials ϕ_i that are solution of the transformed system of Kirchhoff's equations are still a solution of the original system.

Using ENR given by equations (8, 10), we can eliminate sites one by one from the system reducing it to the sites with potentials $\phi_{\rm b}$ that are fixed by boundary conditions. Thus in the Introduction we considered the boundary conditions $\phi_{\rm b} = 0$ for all "boundary" sites "b" while the external field is included in the internal EMFs. As soon as we know the potentials in the reduced system we can restore the initial system site by site. At each step of inverse ENR procedure we have only one unknown variable, namely, the potential of the site being restored. This potential can be found easily since all conductivities and EMFs are well defined for any step of the direct ENR and the inverse ENR procedure as well. Thus we can find potential and current distribution in the system. Then we can calculate effective conductivity $\sigma_{\rm e}$, local field statistics, and all other transport properties of the system. The transformation of the percolation systems similar to given by equation (8) was considered first in references [13,14].

Consider how the local dissipation changes under the ENR. In general the dissipation Q in the original and renormalized graph might be different. For example, the circular current that flows through the sites "k", " i_1 ", and " i_2 ", where the sites " i_1 " and " i_2 " are neighbours of the decimated site "k", does not remain the same in the renormalized system since the loop " $k - i_1 - i_2$ " is decimated from the system together with site "k". In Appendix B we calculate the difference in the dissipation in the original and renormalized system. We obtain that the difference ΔQ_k due to decimating the site "k" is nonzero in general and it is determined by the local conductivities and EMFs. It is important to note that the dissipation ΔQ_k is intrinsic quantity that does not depend on the local potentials ϕ_i . Therefore, we can find the dissipation ΔQ_k even we don't know a priori the potential distribution in the system.

To find the total, bulk dissipation we remove one site at a time from the system. At each step of the ENR procedure the conductivities and EMFs change, but the difference in dissipation before and after removing a site "k" is still given by equation (B.15). Certainly, in the calculating the dissipation ΔQ_k we should use the values of local conductivities and EMFs, which system ascribes at previous stage of ENR, that is those that appear after decimation of k-1 sites from the system. After elimination of all sites the dissipation Q in the system can be calculated as sum of ΔQ_k at each step of renormalization:

$$Q = \sum_{k=1}^{N} \Delta Q_k \tag{12}$$

where N is the total number of sites. Assuming that external field E_0 is uniform and there are not intrinsic EMFs in the original system it is easy to show [2] that bulk dissipation Q is determined by effective conductivity $\sigma_{\rm e}$, namely,

$$Q = \sigma_{\rm e} E_0^2 V, \tag{13}$$

where V is the system volume. Therefore, the ENR method allows us to calculate the dissipation Q, and, therefore the effective conductivity $\sigma_{\rm e}$ without actual calculation of the potential and current distribution, just by decimation sites one by one from the system.

3 Energy dissipation in a Sierpinskii Gasket

To illustrate the ENR method we consider a renormalization of the simple self-similar fractal known as a Sierpinskii Gasket [3,15]. The construction of a 2d Gasket is shown in Figure 1, its fractal dimension $d_{\rm f} = \ln 3/\ln 2$. We set the length of the bond in the elementary triangle is equals to a_0 . All bonds in the fractal are assume to have the same conductivity σ_0 . We wish to determine

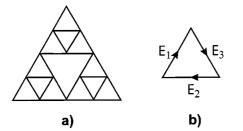


Fig. 1. (a) Sierpinskii gasket of the size $4a_0$, (b) electromotive forces (EMFs) $\mathbf{E} = \{E_1, E_2, E_3\}$, in a single cell of the Sierpinskii gasket.

the energy dissipation Q in the Sierpinskii Gasket as a function of its size L. An uniform fractal is considered where EMFs are the same for each elementary triangle and are described by the vector $\mathbf{E}_0 = \{E_{01}, E_{02}, E_{03}\}$. The positions and directions of EMF E_{01} , E_{02} , and E_{03} are shown in Figure 1b. To calculate the energy dissipation in the Sierpinskii Gasket of size $L = a_0 2^n$ we will consider this fractal as an ensemble of fractals of size $2a_0$. We use the ENR method, namely equations (8, 10), to decimate the "internal" sites in each $2a_0$ fractal as it is shown in Figure 2. After removal of all internal sites, $2a_0$ fractal converts to simple triangle with bond conductivities $\sigma_1 = 3/5$ σ_0 and new EMFs given by vector $\mathbf{E}_1 = \{E_{11}, E_{12}, E_{13}\}$. It follows from equation (10), which is used at each step of the decimation, that vectors \mathbf{E}_1 and \mathbf{E}_0 are connected as

$$\mathbf{E}_1 = \hat{M} \mathbf{E}_0, \tag{14}$$

where the matrix \hat{M} has eigenvalues $\lambda_1 = 2$, $\lambda_2 = 2$, and $\lambda_3 = 3/5$. The eigenvectors for eigenvalues λ_1 and λ_2 can be chosen as $\mathbf{e}_1 = \{1, 0, -1\}/\sqrt{2}$ and $\mathbf{e}_2 = \{1, -2, 1\}/2$ while the eigenvector $\mathbf{e}_3 = \{1, 1, 1\}/\sqrt{3}$ corresponds to the eigenvalue λ_3 . Note that the eigenvector \mathbf{e}_3 represents the circular electric field in the Sierpinskii gasket. The difference in dissipation $\Delta \tilde{Q}_1$ between the fractal of size $2a_0$ and the triangle, which results from its renormalization, can be calculated from equation (B.15), namely,

$$\Delta \tilde{Q}_1 = \frac{116}{125} \left(E_{01} + E_{02} + E_{03} \right)^2 \sigma_0 = 3 \frac{116}{125} \left(\mathbf{e}_3 \cdot \mathbf{E}_0 \right)^2 \sigma_0.$$
(15)

The difference in the dissipation ΔQ_1 between the original fractal and the one where the all internal sites in $2a_0$ fractals are removed is equal to $\Delta Q_1 = \Delta \tilde{Q}_1 (L/2a_0)^{d_f}$. As the next step of transformation we remove the internal sites in $4a_0$ fractals converting them again to a simple triangle. We repeat the above outlined ENR procedure until the size $L = a_0 2^n$ of the fractal is achieved and therefore, the fractal is reduced to the single triangle with bond conductivity $\sigma_n = (3/5)^n \sigma_0$ and EMFs equal to $\mathbf{E}_n = M^n \mathbf{E}_0$. The energy dissipation Q has two constituents: A) Dissipation in the final triangle $Q' = \sigma_n (\mathbf{E}_n \cdot \mathbf{E}_n) = \sigma_n \left(\lambda_1^n (\mathbf{e}_1 \cdot \mathbf{E}_0)^2 + \lambda_2^n (\mathbf{e}_2 \cdot \mathbf{E}_0)^2 + \lambda_3^n (\mathbf{e}_3 \cdot \mathbf{E}_0)^2\right)$, where $\lambda_1 = \lambda_2 = 2$ and $\lambda_3 = 3/5$ are eigenvalues of the matrix M; in the limit $n \to \infty$ the dissipation Q' takes

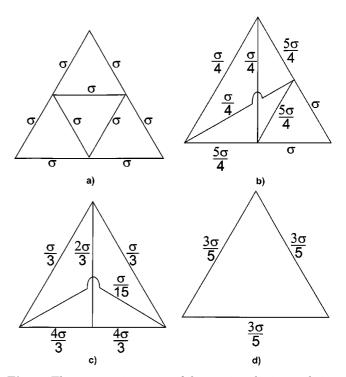


Fig. 2. Three successive steps of decimation the internal sites in $2a_0$ triangle of the Sierpinskii gasket are shown. Current values of the bond conductivities are denoted for each step of exact numerical renormalization (ENR) transformation.

the form $Q' = \sigma_0 (12/5)^n \left((\mathbf{e}_1 \cdot \mathbf{E}_0)^2 + (\mathbf{e}_2 \cdot \mathbf{E}_0)^2 \right)$ since $\lambda_3 < 1$. B) A sum of all "internal" dissipations $\Delta Q = \Delta Q_1 + \Delta Q_2 + \dots + \Delta Q_n$, where

$$\Delta Q_k = \frac{116}{125} \left(\frac{9}{125}\right)^{k-1} \left(\mathbf{e}_3 \cdot \mathbf{E}_0\right)^2 \sigma_0 \left(\frac{L}{a_0}\right)^{d_{\mathrm{f}}}.$$
 (16)

The sum of the internal dissipations ΔQ takes the form $\Delta Q = \sum_{k=1}^{n} \Delta Q_k = \sigma_0 (\mathbf{e}_3 \cdot \mathbf{E}_0)^2 L^{d_{\mathrm{f}}}$ in the limit $n \to \infty$. The total dissipation Q(L) in the fractal of the size L equals to

$$Q(L) = Q'(L) + \Delta Q$$

= $\sigma_0 \left[\left(\left(\mathbf{e}_1 \cdot \mathbf{E}_0 \right)^2 + \left(\mathbf{e}_2 \cdot \mathbf{E}_0 \right)^2 \right) \left(\frac{L}{a_0} \right)^{\frac{\ln(12/5)}{\ln 2}} + \left(\mathbf{e}_3 \cdot \mathbf{E}_0 \right)^2 \left(\frac{L}{a_0} \right)^{\frac{\ln 3}{\ln 2}} \right].$ (17)

The second term in equation (17) increases with L faster than first one. Therefore, the dissipation in the Sierpinskii Gasket is determined mostly by the circular-mesh currents in the fractal. The dissipation of the mesh currents is determined in turn by the smallest loops.

Consider now the Sierpinskii Gasket where the applied field \mathbf{E}_0 is such that $(\mathbf{e}_3 \cdot \mathbf{E}_0) \propto E_{01} + E_{02} + E_{03} = 0$, *i.e.* the sum of the EMFs is equal to zero for all possible contours in the original fractal. There are no mesh current in a such fractal and the dissipation $Q(L) = \sigma_0 E_0^2 (L/a_0)^{-\tilde{t}} (L/a_0)^2$, where the critical exponent $\tilde{t} = \ln (5/3) / \ln 2$, that is, we regain the known result for the effective conductivity [3]. Thus we obtain an important result that the dissipation in the Sierpinskii Gasket essentially depends on the distribution of the local EMF. We speculate that this result holds for any inhomogeneous system though the connection between local field distribution and energy dissipation might be different from the simple equation (17). The energy dissipation is determined by the effective conductivity for the very special case of the EMF distribution only.

4 Bond percolating system near the percolation threshold

We use the above developed ENR method to calculate the effective conductivity of a percolating composite near the percolation threshold. We consider the bond percolation problem determined on a cubic lattice. Each bond of the cubic lattice can be either conducting with the probability p or broken with probability 1 - p. The conducting bonds have the same conductivity σ , conductivity of the broken bonds is equal to zero. We are interested in the bulk effective conductivity $\sigma_{\rm e}$ as a function of the metal concentration p. For the concentration p = 1 the effective conductivity $\sigma_{\rm e}$ coincides with σ . With decreasing p the effective conductivity $\sigma_{\rm e}$ decreases and it vanishes at the concentration $p = p_{\rm c}$ known as the percolation threshold. For concentration p smaller than the percolation threshold $p_{\rm c}$ the effective conductivity $\sigma_{\rm e} = 0$, and the system is dielectric. Therefore, a metal-dielectric transition takes place at $p = p_c$ [1–3]. The recent calculations [16] of the percolation threshold give $p_{\rm c} = 0.2488126 \pm 0.000\,000\,5$.

We consider in detail the effective conductivity $\sigma_{\rm e}$ for the most interesting case when the concentration p of the conducting component is close to the percolation threshold $p_{\rm c}$. To find the local field and current distribution and, therefore, the effective conductivity $\sigma_{\rm e}$ we solve Kirchhoff's equations (3) where ϕ_k are potentials of the sites of the cubic lattice. We choose the external electric field \mathbf{E}_0 in the form $\mathbf{E}_0 = \{E_0, E_0, E_0\}$, so the electromotive forces E_{kj} in equation (3) are equal to $E_{kj} = E_0$ for the bonds coming from a site in +x, +y, and +z directions, while $E_{kj} = -E_0$ for the bonds exiting the site k in -x, -y, and -z directions (see Appendix A). Introduction of the external electric field by EMFs included in all conducting bonds allows us to set cycle boundary conditions in all directions reducing the finite size effects. We are interested in the effective conductivity $\sigma_{\rm e}$ defined as a ratio between applied field and averaged current $(\langle j_x \rangle + \langle j_y \rangle + \langle j_z \rangle)/3 = \sigma_e E_0$. For the bond percolating problem determined on $N \times N \times N$ cubic lattice the current averaging takes the following form

$$\frac{1}{3N^3} \sum_{\langle i,j \rangle} j_{ij} = \sigma_{\rm e} E_0, \qquad (18)$$

where j_{ij} given by equation (4) is the current flowing in-between the sites *i* and *j*, while the summation in equation (18) is going over all $3N^3$ bonds $\langle i, j \rangle$ in the cubic lattice. Note that currents j_{ij} are equal to zero in the broken bonds. Alternatively the effective conductivity can be determined *via* the dissipation Q (see, *e.g.*, [2]), namely,

$$\frac{Q}{3N} = \frac{1}{3N^3\sigma} \sum_{\langle i,j \rangle} j_{ij}^2 = \sigma_{\rm e} E_0^2.$$
⁽¹⁹⁾

In both cases we are interested in the statistical limit $N \to \infty$.

To find the effective conductivity $\sigma_{\rm e}$ we renormalized the percolating system using the ENR method described in the previous section, that is we remove sites one by one, from the system and calculate the dissipation ΔQ_k connected to the currents flowing through the decimated site by means of equation (B.15). Since we use full cyclic boundary conditions we just remove all the sites from the system. When all the sites are eliminated by means of the ENR procedure, we obtain the full dissipation and the effective conductivity $\sigma_{\rm e}$ by equations (12, 19) correspondingly.

For evaluation of the critical exponent t we use the finite-size technique [3,17–19]. Let us consider the critical region of the concentrations p in a vicinity of the percolation threshold p_c , where the percolation correlation length $\xi_{\rm p} \sim |p - p_c|^{-\nu_{\rm p}}$ much larger than unity, here $\nu_{\rm p} \simeq 0.88$ is the critical exponent [3]. For the system size $L \ll \xi_{\rm p}$ the effective conductivity depends only on L, and therefore must be a power of L,

$$\sigma_{\rm e}\left(L\right) = AL^{-t/\nu_{\rm p}}.\tag{20}$$

For L of order of $\xi_{\rm p}$ or larger, additional dependence on L must appear only through the scaling ratio $L/\xi_{\rm p}$ (*i.e.*, $\xi_{\rm p}$ is our only "measuring stick"). Thus the following scaling form is written

$$\sigma_{\rm e} = L^{-t/\nu_{\rm p}} f_1(L/\xi_{\rm p}) = L^{-t/\nu_{\rm p}} f(L^{1/\nu_{\rm p}}(p-p_{\rm c})). \quad (21)$$

In our simulations we take the concentration $p = p_c$ and calculate $\sigma_e(L)$ as a function of the size L. The critical exponent t/ν_p is obtained when equation (20) fitted to numerical data.

The value of the percolation threshold p_c is known, certainly, within some limits of error Δp_c . Therefore, the argument $x = L^{1/\nu_p} \Delta p_c$ of the scaling function f in equation (21) will more and more deviate from zero with increasing L for the chosen numerical value of p_c . As a result equation (20) may not holds in the limit of large L. To check such a potentiality we find the scaling function f(x) in equation (21) by calculating the effective conductivity σ_e for different sizes L and concentration p in the vicinity of the percolation threshold. Thus obtained scaling function f(x) is shown in Figure 3. The data for different sizes L = 4, 8, 16, 32, 64, 128 collapse on the single curve in agreement with finite size scaling. The function can be approximate as $f(x) \approx A + Bx + Cx^2 + Dx^3$, where

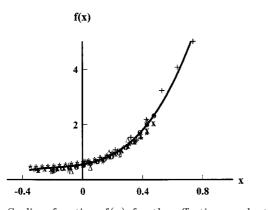


Fig. 3. Scaling function f(x) for the effective conductivity defined by equation (20), $x = L^{\nu_{\rm p}}(p-p_{\rm c})$. Points are numerical results for different sizes $L: (\triangle) \ L = 128$, $(\sharp) \ L = 64$, $(+) \ L = 32$, $(\circ) \ L = 16$, $(\times) \ L = 8$, $(*) \ L = 4$; continuous line is analytical approximation.

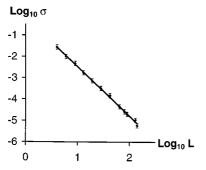


Fig. 4. Effective conductivity σ of 3d bond percolating system as a function on the size L. Concentration of the conducting bonds corresponds to the percolation threshold $p = p_c = 0.2488126$.

A = 0.56, B = 0.98, C = 3.1, D = 5.65 as it is shown in Figure 3.

The percolation threshold is known now with good accuracy, so error Δp_c does not exceed $\Delta p_c \simeq 5 \times 10^{-7}$ [16]. Therefore, even for the largest size L = 140 used in the calculation the critical exponent t the deviation x from zero $\Delta x = L^{1/\nu_p} \Delta p_c$ does not exceed 10^{-4} and deviation the scaling function $f(\Delta x) - f(0)$ is also about 10^{-4} , which is much less than the relative statistical error in calculated values of the effective conductivity $\sigma_e(L)$. Therefore we can use equation (20) to approximate the numerical results.

The results for $\sigma_{\rm e}(L)$ at the percolation threshold are shown in Figure 4. The number of trials for the size L = 4, 6, 9, 13, 19, 28, 42, 64, 80, 90, 128, and 140 were 3500, 2333, 1555, 1076, 736, 500, 333, 218, 175, 155, 109, and 80 respectively. Fitting these results with equation (20) we obtain $t/\nu_{\rm p} = 2.305(15)$. Our value for $t/\nu_{\rm p}$ is in marginal agreement but somehow larger than the values $t/\nu_{\rm p} = 2.2(1)$ of Derrida, Stauffer, Herrmann and Vannimenus [20], $t/\nu_{\rm p} = 2.26(4)$ of Normand and Herrmann [21], $t/\nu_{\rm p} = 2.276(12)$ of Gingold and Lobb [22], and $t/\nu_{\rm p} = 2.282(5)$ by Batrouni, Hansen and Larson [23]. Note that our largest system size $L_{\rm max} = 140$ is almost

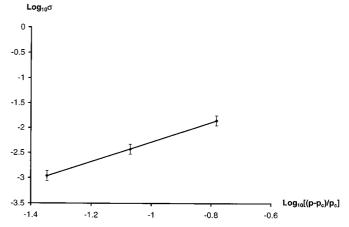


Fig. 5. Conductivity σ of 3d bond percolating system as a function of proximity to percolation threshold $(p - p_c)/p_c$.

twice as large as that having $L_{\text{max}} = 80$ in reference [23]. Our error estimates, like those of references [22, 23], are purely statistical. We did not do a finite-size scaling analysis because, for the large system sizes we used, finite-size effects were so small we could not observe them over the statistical noise in our data. With $\nu_{\rm p} \simeq 0.88$, we therefore, have that $t \simeq 2.0$. To verify this result we also have calculated the effective conductivity $\sigma_{\rm e}(p)$ as a function for the concentration p for the concentrations close to the percolation threshold $p \gtrsim p_{\rm c}$. The conductivity $\sigma_{\rm e}(p)$ for the cubic lattice $80 \times 80 \times 80$ shown in Figure 5 follows the equation $\sigma_{\rm e}(p) = B \left(p - p_{\rm c} \right)^t$ with rather good accuracy when the critical exponent t is chosen to be t = 2.02(2)and numerical factor $B \simeq 0.4$. The value t = 2.0 coincide with upper boundaries for the percolating conductivity exponent t < 2 suggested in reference [9]. It could be speculated [24] that t = 2 is exact result for 3d percolating composites.

5 Discussion and conclusions

Let us now consider qualitatively how the ENR procedure works for a system at percolation threshold when the infinite conducting cluster is much ramified and been approximated by has self-similar blob-link structure [14, 15, 28, 29]. When we eliminate a site from the system by ENR, the number of neighbours for the other sites increases in general, since the sites connected to the decimated site become hold to each other in general. In a regular lattice the ENR procedure will result in an exponential increase of the bonds per site. Therefore, the number of operations (and computer time) to decimate a site increases exponentially in the process ENR. The situation might be different near the percolation threshold due to the characteristic blob-link structure of the infinite percolating cluster. Consider a blob with size \mathcal{L} consisting of multi-connected sites and suppose that the blob is connected to the rest of the percolating system by two bonds only. If we decimate all sites of the blob but one, this last site has two neighbours. Note that this result of ENR does not depend on the internal structure of the eliminated blob. We can apply ENR to all blobs of size \mathcal{L} , reducing each of them to one site. If the backbone of the infinite cluster has a self-similar structure the resulting structure repeats the structure of the initial backbone, but the distance between new sites increases from 1 to \mathcal{L} . At the next steps of ENR, we can eliminate blobs of size \mathcal{L}^2 and so on, until the size L of the whole system is achieved.

If the number of bonds per site does not increase then the ENR procedure requires L^d operations only to decimate all the sites from a percolating system of size L and dimensionality d, and, consequently, to calculate its effective conductivity. We can compare this estimate with the number of operations in other exact methods: the transfer matrix method [25] takes about L^7 operations, Frank Lobb algorithm [26] takes L^4 operations but this algorithm works for 2d systems only. For example, the ENR procedure takes about five minute on a Pentium 400 computer to calculate the effective conductivity of a percolating system with size $140 \times 140 \times 140$ and concentration $p = p_{\rm c}$. Note that the ENR procedure has a disadvantage since it works with above efficiency for the concentrations p close to the percolation threshold. Still ENR may be very useful for simplification of the percolating system even far away from the percolation threshold since it eliminates the isolated clusters and increases sharply the connectedness of the system. After these simplifications, rather effective relaxation methods [27] can be used to calculate conductivity as has been done in reference [12].

The question of whether there is a fixed point for the ENR transformation at the percolation threshold now arises. Suppose we divide the system in blocks of size \mathcal{L} and then use ENR to decimate all sites in each block but one. Then we repeat the procedure: we divide the system resulting from previous ENR on the blocks of size \mathcal{L}^2 and again decimating all sites but one in each block of the size \mathcal{L}^2 . We repeat this block ENR again and again. There are in general two possible scenarios for the system transformation under successful block ENR. In the process of transformation the system may take the form of some self-similar fractal like the Sierpinskii Gasket and will not change further except all the distances will scale like $L = \mathcal{L}^k$, where k is the number of transformations. But it is now clear that the infinite cluster and the backbone are not hierarchical. It follows from, e.g., the current probability distribution, which is not log normal, as would be in the case for a hierarchical lattice [30,31]. To see how does the structure of the percolation system changes under ENR transformation have computed the average distance *l* between the sites in the process of the block reduction as

$$l(L) = \frac{1}{\mathcal{L}^k N_{\rm b}^{(k)}} \sum_{i>j} l_{ij}^{(k)}, \qquad (22)$$

where $l_{ij}^{(k)}$ is the length of the bond between sites "i" and "j" that appears after the blocks of size $L = \mathcal{L}^k$ are reduced to the single sites, $N_{\rm b}^{(k)}$ is the total number of

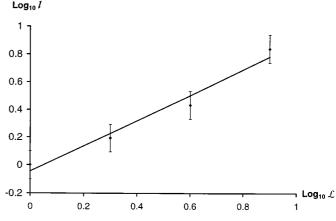


Fig. 6. Average distance l between connected sites as a function of block size \mathcal{L} . The distance is measured in terms of \mathcal{L} .

conducting bonds after k ENR transformations. The length l(L) can be thought as a radius of interaction in the system (measure of nonlocality). The radius of interaction l(L) would achieve a fixed value l_c for $L \to \infty$ if the ENR transformations have a fixed point. The result of our calculations shown in Figure 6 does not confirm this suggestion. The system does not remain the same in the process of ENR. The radius of interaction l(L) increases gradually as

$$l(L) \propto L^{\alpha}, \tag{23}$$

where the exponent α might be estimated as $\alpha \simeq 0.9$. We do not see any saturation of l(L) with increasing the size L. This result confirm that system is not self similar at the percolation threshold so that its structure changes gradually in the course of the ENR transformations.

In conclusion, we present detail description of a numerical method for calculation of the transport phenomena in macroscopically inhomogeneous media. Our method of exact numerical renormalization (ENR) can be applied to any macroscopically inhomogeneous media, but it is most successful if the transport problem is defined on a self-similar or quasi-selfsimilar structure. We show this by considering the internal dissipation in the Sierpinskii Gasket and the effective conductivity of 3d percolating system. In the last case the ENR method allows us to calculate conductivity at the percolation threshold using only a Pentium PC for a system whose size previously require a super computer [23]. Far away from the percolation threshold the ENR method does not allow us to obtain explicitly the effective transport properties. Yet it can be used to sufficiently simplify the system, namely to reduce its criticality, so that other computer methods like relaxation can be used successfully.

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Appendix A: Kirchhoff's equations as a model for a composite medium

In this Appendix we show how the charge conservation law given by equation (1) can be reduced to the set of Kirchhoff's equations (3). That is we show the transport properties of a composite medium can be modeled by a discrete electric circuit. Let us assume that an imaginary cubic lattice with period Δ is immersed in the inhomogeneous medium which is characterized by local conductivity $\sigma(\mathbf{r})$. Then we can rewrite equation (1) in a discrete form. The vertexes of the lattice are numbered with three integer numbers, *i.e.*, a vertex with coordinates $\mathbf{r} = \{l\Delta, m\Delta, n\Delta, \}$ has the numbers $\{l, m, n\}$. Thus we obtain instead of partially differential equation (1) the following set of the linear equation determined at each site of the cubic lattice

$$\begin{split} &-\frac{1}{\Delta} \begin{bmatrix} \sigma \left(l+1/2,m,n \right) \frac{\phi \left(l+1,m,n \right) - \phi \left(l,m,n \right) }{\Delta} \\ &-\sigma \left(l-1/2,m,n \right) \frac{\phi \left(l,m,n \right) - \phi \left(l-1,m,n \right) }{\Delta} \end{bmatrix} \\ &+ \frac{E_{0x}}{\Delta} \left[\sigma \left(l+1/2,m,n \right) - \sigma \left(l-1/2,m,n \right) \right] \\ &- \frac{1}{\Delta} \begin{bmatrix} \sigma \left(l,m+1/2,n \right) \frac{\phi \left(l,m+1,n \right) - \phi \left(l,m,n \right) }{\Delta} \\ &- \sigma \left(l,m-1/2,n \right) \frac{\phi \left(l,m,n \right) - \phi \left(l,m-1,n \right) }{\Delta} \end{bmatrix} \\ &+ \frac{E_{0y}}{\Delta} \left[\sigma \left(l,m+1/2,n \right) - \sigma \left(l,m-1/2,n \right) \right] \\ &- \frac{1}{\Delta} \begin{bmatrix} \sigma \left(l,m,n+1/2 \right) \frac{\phi \left(l,m,n+1 \right) - \phi \left(l,m,n \right) }{\Delta} \\ &- \sigma \left(l,m,n-1/2 \right) \frac{\phi \left(l,m,n \right) - \phi \left(l,m,n-1 \right) }{\Delta} \end{bmatrix} \\ &+ \frac{E_{0z}}{\Delta} \left[\sigma \left(l,m,n+1/2 \right) - \sigma \left(l,m,n-1/2 \right) \right] = 0, \quad (A.1) \end{split}$$

where $\phi(l, m, n)$ is the fluctuating potential at the lattice site $\{l, m, n\}$, $\sigma(l + 1/2, m, n)$ is the local conductivity defined in-between the sites $\{l, m, n\}$ and $\{l + 1, m, n\}$, *i.e.* $\sigma(l + 1/2, m, n) = \sigma(\mathbf{r})$, with $\mathbf{r} =$ $\{(l + 1/2) \Delta, m\Delta, n\Delta\}$; conductivities $\sigma(l - 1/2, m, n)$, $\sigma(l, m \pm 1/2, n)$ and $\sigma(l, m, n \pm 1/2)$ are defined in a similar way. We also suppose that the external electric field \mathbf{E}_0 with components $\mathbf{E}_0 = \{E_{0x}, E_{0y}, E_{0z}\}$ is uniform over the composite. We define now the multi-indexes k as $k = \{l, m, n\}$ and rearrange equation (A.1) as

$$\sum_{j} \sigma_{kj} \left(\phi_j - \phi_k \right) - \Delta \sum_{j > k} \sigma_{kj} E_j + \Delta \sum_{j < k} \sigma_{kj} E_j = 0,$$
(A.2)

where j is another multi-index which denotes the nearest neighbours of the site k; the first sum in equation (A.2) is over all nearest neighbours; the second sum is over "j > k", *i.e.*, the multi-index j takes values $j_1 = \{l + 1/2, m, n\}, j_2 = \{l, m + 1/2, n\}$ or $j_3 =$ $\{l, m, n + 1/2\}$; the third sum is over "j < k", *i.e.*, the multi-index j takes values $j_4 = \{l - 1/2, m, n\}, j_5 =$ $\{l, m - 1/2, n\}$ or $j_6 = \{l, m, n - 1/2\}$; the components E_j of the external fields take values $E_{j_1} = E_{0x}$, $E_{j_2} = E_{0y}$, $E_{j_3} = E_{0z}$ in the second sum and E_j takes values $E_{j_4} = -E_{0x}$, $E_{j_5} = -E_{0y}$, $E_{j_6} = -E_{0z}$ in the third sum in equation (A.2); the conductivities σ_{kj} are equal to the local conductivity $\sigma(\mathbf{r})$ in-between the sites k and j. If we define the electromotive force E_{kj} as $E_{kj} = -\Delta E_j$ for k > j and as $E_{kj} = \Delta E_j$ for k < j then equation (A.2) takes the form

$$\sum_{j} \sigma_{kj} \left(\phi_j - \phi_k + E_{kj} \right) = 0, \qquad (A.3)$$

which coincides with Kirchhoff's equations (3). The solution of equations (A.3) tends to the potential distribution given by equation (1) in the limit $\Delta \to 0$.

We use a cubic lattice to discrete the inhomogeneous media and obtain equations (A.3). The above consideration can be repeated for any spatial lattice. As a result we will again get Kirchhoff's equations determined on a particular lattice, though the values of σ_{kj} and E_{kj} might be different from obtained for the square lattice. Moreover, we do not need a regular lattice at all. When the conducting phase has rather ramified spatial distribution, as takes place in brine saturated rocks, very sophisticated triangulations are used in order to discretize the system and solve the conductivity or flow problem (see, *e.g.*, [4]).

Note that most of the theoretical works on percolation have actually dealt with random resistor networks, where conductivities σ_{kj} are assumed to be statistically independent, rather than with continuum composites. In the spirit of the modern theory of critical phenomena it is assumed that the important critical properties are universal, *i.e.*, independent of the precise details of the model-like correlation in values of σ_{kj} (see discussion in [2]).

Appendix B: Change in dissipation under ENR transformation

In this Appendix we calculate the difference in the dissipation in the original and renormalized system where the site "k" is decimated. To simplify the straightforward but somehow tedious calculations we introduce the following variables

$$\varepsilon_{ij} = E_{ij} + \phi_j - \phi_i \tag{B.1}$$

$$\varepsilon_{ii}' = E_{ii}' + \phi_i - \phi_i \tag{B.2}$$

$$\varepsilon_{ij}^* = E_{ij}^* + \phi_j - \phi_i$$
 (B.3)

where "i" and "j" are sites, connected to the site "k" decimated from the system, while EMFs E'_{ij} and E^*_{ij} are given by equations (11, 10) respectively. The quantities ε_{ij} , ε'_{ij} , and ε^*_{ij} are not independent. Substituting the expression for E^* given by equation (10) in equation (B.3) and using equation (8) we obtain

$$\varepsilon_{ij}^* = \frac{1}{\sigma_{ij}^*} \left(\sigma_{ij} \varepsilon_{ij} + \sigma'_{ij} \varepsilon'_{ij} \right)$$
(B.4)

where conductivities σ_{ij}^* and σ_{ij}' are given by equations (8, 9) respectively.

The total dissipation of the energy Q in the original system is equal to

$$Q = \sum_{m,n < m} \sigma_{mn} \varepsilon_{mn}^2, \tag{B.5}$$

where the summation is over all sites of the graph. Since the ENR procedure changes the conductivities and EMFs of the neighbours of the decimated site "k" only, the difference in the dissipation before and after the decimation of the site "k" can be written in the following form

$$\Delta Q_k = \sum_i \sigma_{ki} \varepsilon_{ki}^2 + \sum_{i,j < i} \sigma_{ij} \varepsilon_{ij}^2 - \sum_{i,j < i} \sigma_{ij}^* \varepsilon_{ij}^{*2} \qquad (B.6)$$

where the summation goes over the sites "i" and "j" connected to the decimated site "k", and ε_{ij} , ε_{ij}^* , and σ_{ij}^* are given by equations (B.1, B.3, 8) respectively. Note, that the last term in equation (B.6) is the sum of the dissipations in the bonds between sites "i" and "j" that are renormalized by the ENR procedure applied to the site "k". Substituting equation (B.6) in equation (B.4) for the renormalized ε_{ij}^* and using then equations (8, 9) we rewrite equation (B.6) as

$$\begin{aligned} \Delta Q_k &= \sum_i \sigma_{ki} \varepsilon_{ki}^2 - \sum_{i,j(j

$$(B.7)$$$$

To simplify equation (B.7) we separate out the difference $\varepsilon'_{ij} - \varepsilon_{ij}$ in the parentheses, obtaining

$$\Delta Q_k = \sum_i \sigma_{ki} \varepsilon_{ki}^2 + \sum_{i,j \ (j < i)} \frac{\sigma'_{ij} \sigma_{ij}}{\sigma_{ij}^*} \left(\varepsilon'_{ij} - \varepsilon_{ij} \right)^2 - \sum_{i,j \ (j < i)} \sigma'_{ij} \varepsilon'_{ij}^2.$$
(B.8)

Let's demonstrate that the first and the last sums in equation (B.8) cancel each other. Indeed, substituting equation (11) in equation (B.2) and using equation (B.1) we can see that $\varepsilon'_{ij} = \varepsilon_{ik} + \varepsilon_{kj}$. From this equation and equation (9) it follows that the last sum in equation (B.8) can be written as

$$\sum_{i,j \ (j < i)} \sigma'_{ij} \varepsilon'^{2_{ij}} = \frac{1}{\sum_{n} \sigma_{kn}} \sum_{i,j \ (j < i)} \sigma_{ik} \sigma_{kj} \left(\varepsilon_{ik} + \varepsilon_{kj}\right)^2,$$
(B.9)

where the summation in the denominator goes over all neighbours of the site "k". We use the relations $\sigma_{ik} = \sigma_{ki}$ and $\varepsilon_{ik} = -\varepsilon_{ki}$, that follows from definition ε_{ik} given by equation (B.1) and the "vector" properties of EMF

 $E_{ik} = -E_{ki}$ (see Appendix A) to present equation (B.9) in a "symmetric" form, namely,

$$\sum_{i,j \ (j(B.10)$$

Neither of the two terms in the square brackets changes under the exchange indexes "i" and "j". This symmetry allows us to extend the summation in equation (B.10) over all values of the indexes "i", "j". Thus, we obtain

$$\sum_{i,j \ (j < i)} \sigma'_{ij} \varepsilon'^{2}_{ij} = \frac{1}{\sum_{n} \sigma_{kn}} \frac{1}{2} \left[2 \sum_{i,j} \sigma_{ik} \sigma_{kj} \varepsilon^{2}_{ik} -2 \left(\sum_{i} \sigma_{ki} \varepsilon_{ki} \right) \left(\sum_{j} \sigma_{kj} \varepsilon_{kj} \right) \right]$$
$$= \sum_{i} \sigma_{ik} \varepsilon^{2}_{ik} - \left(\sum_{i} \sigma_{ki} \varepsilon_{ki} \right)^{2} \frac{1}{\sum_{n} \sigma_{kn}}, (B.11)$$

where all the summations are still over the sites that are connected to the decimated site "k".

Note, we assume there is no connection of a site with itself, *i.e.*, we assume that $\sigma_{ii} = 0$ and $E_{ii} = 0$ for all the sites in the original system. It is easy to verify that the "loop" connections will not appear in the course of the ENR procedure and, therefore, σ_{ii} , E_{ii} , and ε_{ii} remain zero after an arbitrary number of decimations. We show now that the last term in equation (B.11) is exactly equal to zero. Substituting in the sum $\sum_i \sigma_{ki} \varepsilon_{ki}$ expression for ε_{ik} from equation (B.1) we obtain the equation

$$\sum_{i} \sigma_{ki} \varepsilon_{ki} = \sum_{i} \sigma_{ki} \left(\phi_i - \phi_k + E_{ki} \right), \qquad (B.12)$$

which coincides with Kirchhoff's equation (3) for the site "k". Therefore, the sum $\sum_i \sigma_{ki} \varepsilon_{ki}$ is equal to zero. Substituting this result in equation (B.11) we obtain that

$$\sum_{i,j \ (j$$

which means that first and third terms in equation (B.8) cancel each other. As a result we get from equation (B.8) a simple equation for the dissipation ΔQ_k :

$$\Delta Q_k = \sum_{i,j \ (j$$

where the summation still goes over the sites "i" and "j" connected to the decimated site "k". Substituting here the definitions of the conductivities σ_{ij}^* , σ_{ij}' and "electric fields" ε_{ij} , ε_{ij}' given by equations (8, 9) and (B.1, B.2)

respectively we obtain the final formula of the dissipation ΔQ_k , namely,

$$\Delta Q_k = \sum_{i,j \ (j < i)} \frac{\sigma_{ik} \sigma_{kj} \sigma_{ij}}{\sigma_{ik} \sigma_{kj} + \sigma_{ij} \sum_n \sigma_{kn}} \left(E_{jk} + E_{ki} + E_{ij} \right)^2$$
(B.15)

where we still use that $E_{ik} = -E_{ki}$ and all sums are over the neighbours of the decimated site "k".

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