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New method for the exact determination of the effective conductivity and the local field in RLC networks

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Abstract. We present a new numerical method for exactly determining the effective conductivity and the local field for random RLC networks. This method is compared with a real-space renormalization group method and the Frank and Lobb (FL) method. Although our method is slower than the FL method, it also exactly computes the local field for large-size systems. We also show that the renormalization group method fails in determining the local field.

1. Introduction

During the last two decades there has been an increasing interest in the optical properties of materials [1, 2]. It seems that the local electromagnetic field and its fluctuations are the main quantities related to various optical processes in composite systems such as Raman scattering [1, 3, 4], Rayleigh scattering [5] and nonlinear optics [1, 6–10], as well as the electromagnetic processes in mesoscopic systems [2]. On the other hand, the large field fluctuations in composite structures were attributed to the localization [11–13]. These field fluctuations were observed in both 3D rough surfaces as well as in 2D metal-dielectric composites at the percolation threshold and for a characteristic frequency ω_{res} (where the conductivities of the components have the same magnitude) [4, 5, 14]. They have also been used to explain the anomalously high absorption observed in the visible, near-infrared and microwave frequencies around the percolation threshold [15].

In most of these investigations the system is modelled into RLC networks by assuming that the plasmon frequency is much larger than the relaxation rate [16]. Some particular properties of such random networks have recently been analytically investigated [17]. Several methods, on the other hand, have been used to determine the local field and the effective conductivity in such networks. There exist fast algorithms such as the Frank and Lobb (FL) method [18] and the transfer matrix method [19], which exactly compute the effective ac and dc conductivities as well as the critical exponents. However, these methods are not useful for the local field calculations. To this end, the most used method in recent years has been the real space renormalization group (RSRG) method [20]. This very fast method has been shown to provide reasonably good approximations for the effective conductivity and the critical exponents [14], and was expected to provide similar results for the local field. However, although its validity

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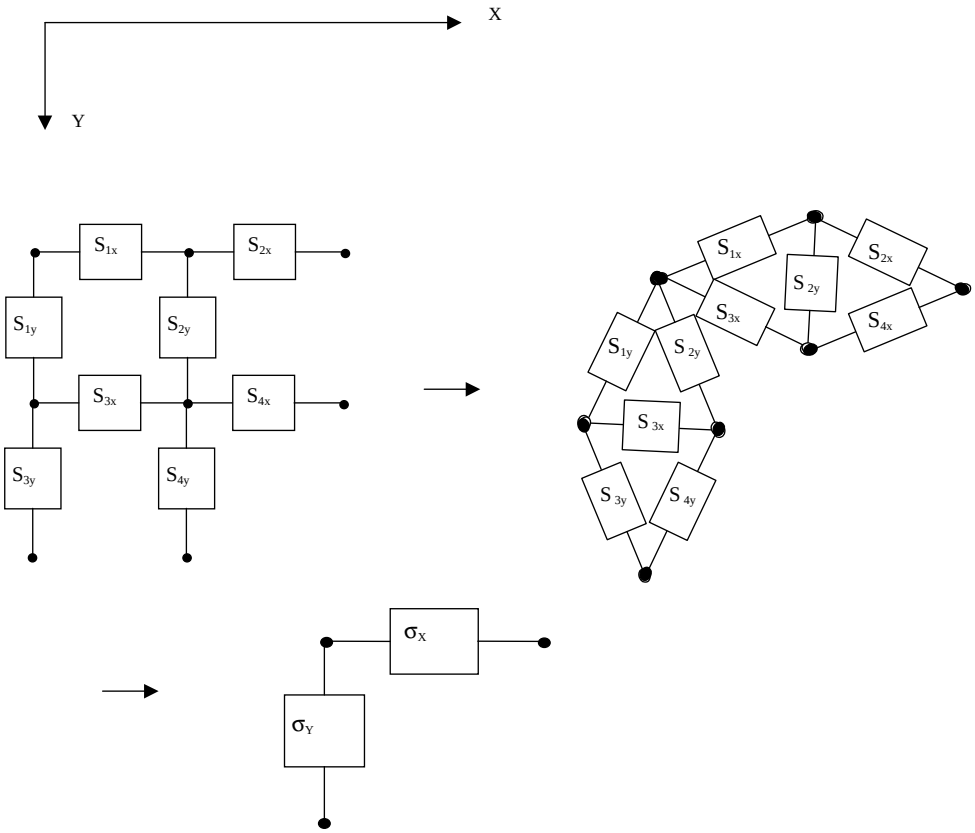

Figure 1. A schematic diagram of the RSRG method.

for the field calculations was not checked, this method has been extensively used to describe the above-mentioned optical processes based on its fluctuations. In fact, this method consists of the transformation of the lattice into Wheatstone bridges which, after a series of transformations, are reduced to only two bonds in the x and y directions (see figure 1). We note here that this transformation into bridges either shunts some bonds (such as S_{1y} in the x direction) or uses others twice (such as S_{2y} in the x and y directions). This may limit the dispersion of the current in the neighbouring branches and then enhances the field which, as a consequence, should be overestimated. However, this method has been used as an alternative since an exact method consists of the resolution of Kirchoff equations which, for large lattices, allows the use of very large matrices ($N^2 \times N^2$ for a system size $N \times N$). Actually, for a sample size of 256×256 we need a matrix of $256^2 \times 256^2$ which uses a memory of about 125 Gb for double-precision complex variables. This amount of memory is currently unavailable in RAM memories or on hard disks.

The aim of this paper is to propose a new method exactly computing, for reasonably large systems of bonds, both the effective conductivity and the local field (site systems can be treated by other methods [1]). Since the field is the quantity that is involved in many physical processes and should be determined exactly, the main objective here is to compute the local field. Section 2 is devoted to the description of the method, while in section 3, we will briefly mention the comparison with the FL method for the dc conductivity and the critical exponents.

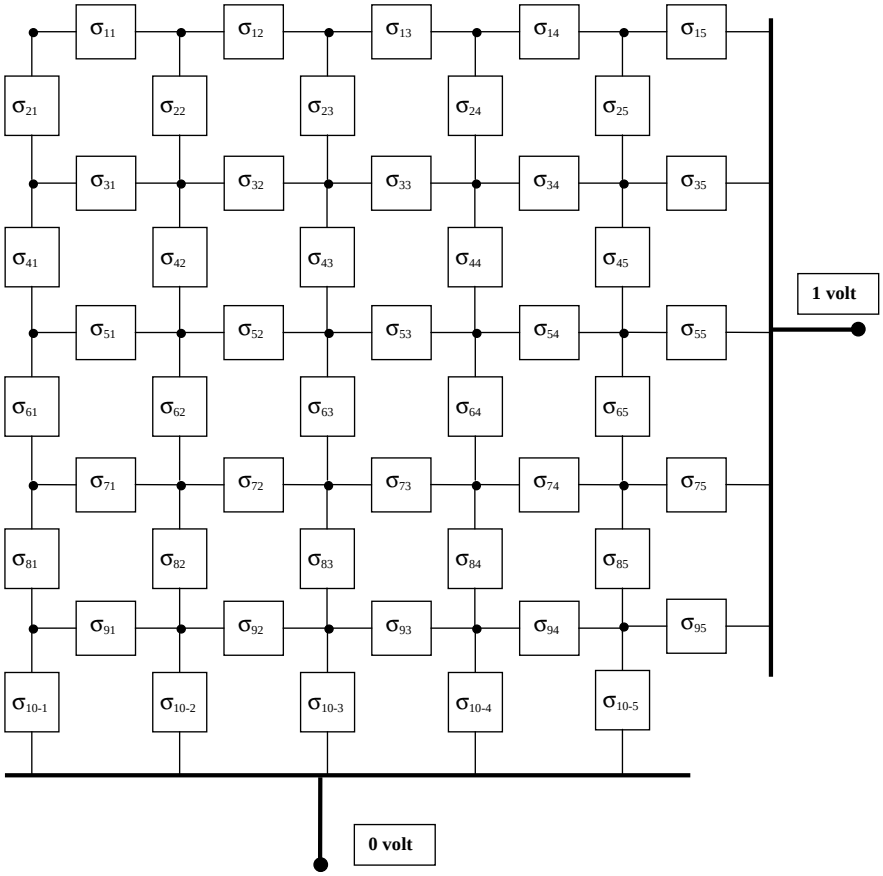

Figure 2. A sample of an L lattice of size 5.

This will be followed by the local field calculations and comparison with the RSRG method. In this section we will also show the field distribution for two different geometries.

2. Description of the method

Let us consider a 2D lattice randomly filled with two different complex conductivities (actually metallic and dielectric ac conductivities with filling concentrations p and $1-p$, respectively). We can extend this method to three dimensions since the same kind of matrices can be used but with different elements. The two ends of the lattice are connected to the ground ($V = 0$ V) and ac voltage V (here $V = 1$ V). In general, two different lattice geometries have been used in this problem: the one shown in figure 2 (used by the RSRG method [20]), in which the two ends are perpendicular (called the L lattice from now on) and the other one shown in figure 3 (used by other methods such as the FL [18] and the transfer matrix methods [19]), in which the ends are parallel (called the PAR lattice from now on). These lattices have different numbers of nodes and bonds. For instance, an L lattice of size N has $2N^2$ bonds and N^2

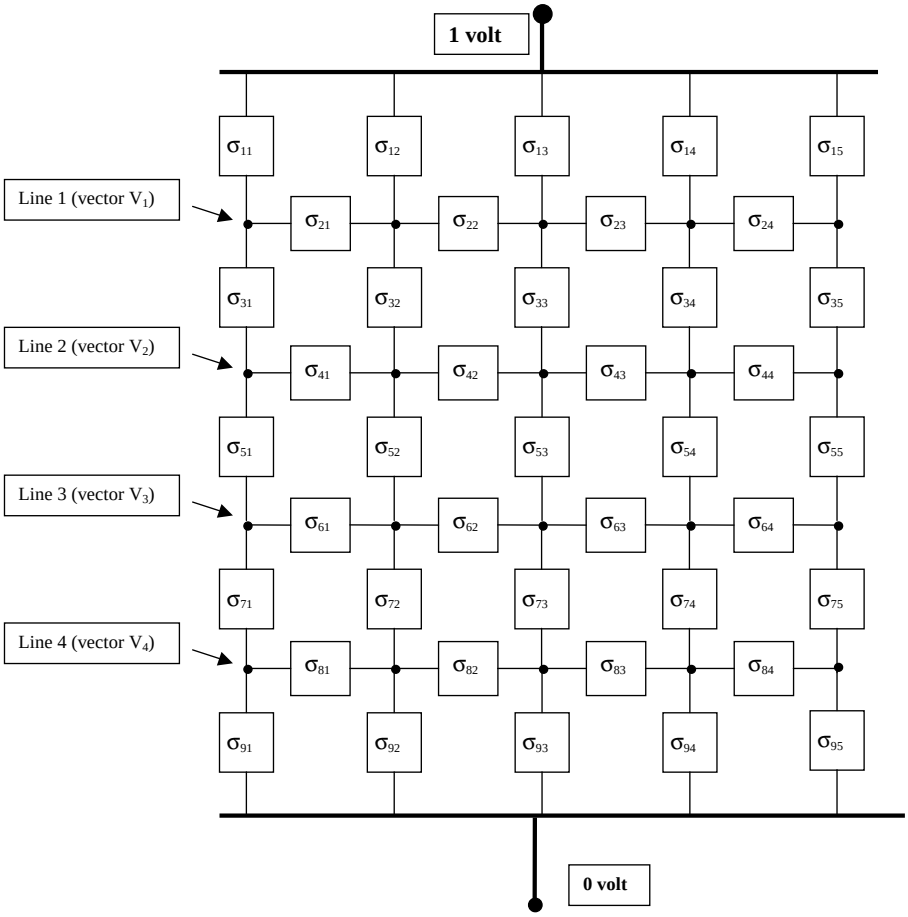

Figure 3. A sample of a PAR lattice of size 5.

nodes, while a PAR lattice of the same size has $N^2 + (N-1)^2$ bonds and $N(N-1)$ nodes as shown in figures 2 and 3, respectively. It is important to note that the percolation threshold for the L lattice should take place for a much smaller concentration than that usually known for 2D lattices (i.e., $p_c = 0.5$) since the two ends (0 and 1 V) can only be connected by two bonds (the ends of the lower line and the right column of the lattice in figure 2) which may constitute an infinite cluster. Indeed, the probability of obtaining such a cluster varies as p^2, and is independent of the lattice size.

In order to determine the local field and the effective conductivity σ_{eff}, which is the current incident to (or outgoing from) the lattice since the voltage is 1 V, we use the Kirchoff equations at each node i, j:

$$\sum_{k,l}(V_{k,l} - V_{i,j})\sigma_{k,l}^{i,j} = 0 \tag{1}$$

where the summation is over the nodes k, l connected to the nodes i, j by the conductivities $\sigma_{k,l}^{i,j}$. For the nodes connected to the 1 V end, we replace the corresponding $V_{k,l}$ by the value 1. We then have M equations ($M = N^2$ for L lattices and $N(N-1)$ for PAR lattices) of M

unknown potentials. We can rewrite equation (1) within its matricial form:

$$\tilde{\Gamma}\vec{V} = \begin{pmatrix} P_{11} & P_{12} & 0 & \cdots & 0 \\ P_{21} & P_{22} & P_{23} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & P_{N-1,N-2} & P_{N-1,N-1} & P_{N-1,N} \\ \cdots & \cdots & 0 & P_{N,N-1} & P_{N,N} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ \cdots \\ V_{N-1} \\ V_N \end{pmatrix} = \begin{pmatrix} S_1 \\ S_2 \\ \cdots \\ S_{N-1} \\ S_N \end{pmatrix}. \tag{2}$$

In this matricial equation, the matrix $\tilde{\Gamma}$ is symmetrical tridiagonal composed of $N \times N$ ($(N-1) \times (N-1)$ for the PAR lattice) block elements $P_{i,j}$, which are themselves matrices of dimension $N \times N$. The $P_{i,j}$ elements appearing in the diagonal region of $\tilde{\Gamma}$ are also symmetrical tridiagonal matrices while those appearing outside this region are diagonal. These matrices consist of combinations of the branch conductivities obtained by equation (1). The vector $\vec{V}$ is composed of N ($N-1$ for PAR lattices) elements V_i, which are themselves vectors of size N corresponding to the potentials in the nodes of the ith line (see figures 2 and 3). The elements S_i are vectors of the same size as V_i. These vectors in the L lattices consist of 0 elements, except the last one which contains the conductivity of the ith line connected to the voltage unity. For PAR lattices, all the vectors S_i, except S_1, are 0 elements. For these lattices, the elements of S_1 contain the conductivities connected to the voltage one.

At first glance, it appears impossible to solve equation (2) for large systems because the handling and storage of the matrix $\tilde{\Gamma}$ requires a huge amount of memory which 'readily available' computers cannot provide. For example, if we consider a lattice size of 256×256 we need a memory of about 125 Gb, as discussed above. In fact, only five sets of elements are not 0 in this matrix, while we need to store only three of them due to symmetry. We then partially re-linearize this equation so that we get the set of N ($N-1$ for PAR lattices) equations using the P matrices:

$$\sum_j P_{i,j} V_j = S_i \tag{3}$$

where i varies between 1 and N (or $N-1$ for PAR lattices). Note here that from the particular configuration of $\tilde{\Gamma}$, each equation uses, at most, three P matrices; the others are 0 matrices. We solve this set of equations by using the substitution method where, starting from the equation for $i = N$, we replace in each step the vector V_i by V_{i-1} up to the equation for $i = 1$, where V_1 is determined. Then we use the inverse procedure to determine the other V_i vectors. This inverse procedure implies the storage of all the combinations of the P matrices involved during the substitution steps. We then store only N matrices of size $N \times N$ and N vectors of size N to solve this set of equations (for PAR lattices the N vectors are not needed). Although the amount of memory required is very large for large systems, it is much less than if we directly use the mother matrix $\tilde{\Gamma}$. For instance, for a sample size of 256×256, the memory required now corresponds to about 250 Mb, which is fairly reasonable. Since the memory used is high, we store the matrices involved in the substitution procedure on hard disk, while the non-zero elements of the P matrices are stored in the RAM memory. For this sample size, we need a RAM memory of about 12 Mb. The computation time spent processing one sample is about 18 min with a simple Pentium II 300 MHz processor. Therefore, with this method it is possible to reach sample sizes as large as 256×256 within a reasonable computation time using a PC computer—a situation which was not possible with the usual exact methods. In order to check our results, we systematically calculated the incident and outgoing currents which are always identical and means that the current is conserved. We also checked the current conservation in each node. The current in the nodes is not conserved in the case of the RSRG method.

3. Comparison with other methods

The present method provides both the effective conductivity and the local field. Concerning the effective conductivity, fast algorithms such as the FL [18] and transfer matrix methods [19] determine it exactly. We compared our calculations for PAR lattices with those of the FL method for the dc conductivities at percolation threshold ($p_c = 0.5$). We found exactly the same effective conductivity for the same sample configurations. The results are identical to those of the FL method up to the last digit of the Fortran precision used. It is obvious that we get the same results as the FL method since this method is also based on the Kirchoff equations for its transformations. However, we should note here that in their paper of 1984 [18], Frank and Lobb showed results claiming that the effective conductivity is averaged up to a very high accuracy (less than 1%), while we found a much lower accuracy (sometimes up to 30%). Indeed, for small-size samples, the number of configurations is small and the average should not be sufficient to reach such an accuracy. They averaged their results for the smallest sizes (e.g., less than 10×10) over 110 000 configurations, but the total number of configurations for these sizes is much smaller and the configurations generated are often the same. We expect the accuracy to become better for sample sizes greater than 200×200. Since we get the same results as the FL method for the effective conductivity, we can also get the same critical exponents.

Now let us consider the local field calculations and compare our results with the RSRG method which seems to be extensively used for the field calculations in bond systems. Here we compare the local field distribution obtained by this method with our method. The sample size used here is 256×256 (for a sample of twice the size, the hard disk space needed is multiplied by eight).

For the rest of this paper we will restrict ourselves to the characteristic frequency ω_{res} where the dielectric and metallic conductivities are of the same magnitude, while the metallic concentration is $p = 0.5$. In this case, the framework $L = C = \omega_{\text{res}} = 1$ has been used [4,5,14] and giant field fluctuations were found within the RSRG method. We use these parameters in this work for the ac case. In this framework, the metallic conductivity is

$$\sigma_m = \frac{1}{i + R} \tag{4}$$

and the dielectric conductivity

$$\sigma_d = i \tag{5}$$

R being the loss in the metallic component (related to the relaxation rate [14, 16]).

In figures 4(*a*)–(*c*) we show, for different R values, the field intensity ($\log |E|^2$) distribution obtained by our method with L lattices (solid curves), PAR lattices (dashed curves) and those obtained by the RSRG method (dotted curves). Recall that the RSRG method is used for L lattices, and that PAR lattices are used to examine the influence of the lattice geometry on the field distribution. In these figures we clearly see that the distribution of the field is log-normal with our method for L lattices and that the peaks at lower strengths appearing in the RSRG curves for different losses do not appear in the same kind of lattice in our method. The high-strength peak, on the other hand, is much larger for the RSRG method. These large values obtained by the RSRG method can be explained by the fact that in the RSRG method some branches are shunted so that the Wheatstone bridge is obtained and renormalization can be performed (see figure 1). Indeed, the maximum field in the RSRG method seems to diverge as $1/R$ for vanishing losses. However, this divergence (which is unphysical) should disappear in a real lattice since the current should be dispersed in the shunted branches.

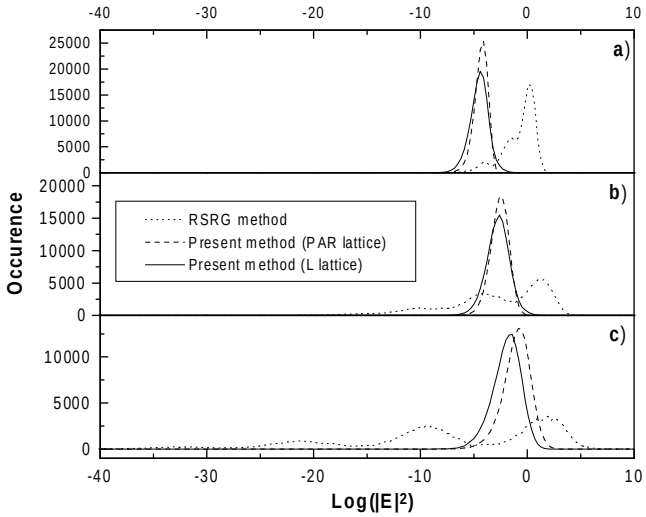

Figure 4. Distribution of the logarithm of the local field strength ($\log|E|^2$) for the present method with an L lattice (solid curves), PAR lattice (dashed curves) and for the RSRG method (dotted curve). (*a*) $R = 0.1$, (*b*) $R = 10^{-3}$, (*c*) $R = 10^{-6}$.

The general shape of the distribution seems to be unaffected by the geometry. Indeed, the field distribution is also log-normal for a PAR lattice. This distribution is slightly wider than that of the L lattice, but the maximum field strength remains much smaller than in the RSRG distribution. Therefore, all the optical processes investigated recently using the RSRG method have overestimated the field fluctuations which significantly affects these processes. Therefore, they should be reinvestigated using this method in order to see the real enhancement of the local field.

4. Conclusion

We have described an exact numerical method determining both the local field and the effective conductivity of RLC networks. Various verifications have been performed to examine the exactness of this method. In particular, it has been shown that this method provides the same effective conductivity as the FL method for dc networks. However, this method needs a large amount of hard-disk memory storage capacity and sensitively increases the computing time. If we consider lattice sizes much larger than 256×256, 'readily available' memory sizes become insufficient; however, this lattice size is already enough to produce good statistical data for the field distribution, as shown in figure 4. The challenge now is to reduce the amount of memory required by using an adequate matricial algebra. This should be the goal of forthcoming works.

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