Real-space renormalization and effective-medium approximation to the percolation conduction problem

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We present a new approach, the renormalized effective-medium approximation (REMA), for the percolation conductivity problem in disordered conductance networks. This approach combines real-space renormalization and effective-medium approximation techniques. We use it to investigate two-, three-, and four-dimensional bond-disordered conductance networks. REMA provides excellent predictions for the network conductivity $g(p)$ over the entire range of fraction p of conducting bonds in two and three dimensions. REMA reproduces the exact bond percolation threshold of the square lattice and predicts bond percolation thresholds for the simple cubic lattices in three and four dimensions which differ only by about 6% and 1%, respectively, from the best available estimates. It also provides good estimates of the conductivity critical exponents t and s in both two and three dimensions.

INTRODUCTION

Random conductance networks have become an important model for the investigation of transport phenomena in disordered materials such as diffusion and conduction in amorphous and inhomogeneous materials and spin-wave properties in disordered ferromagnets.[1] Despite the conceptual simplicity of such models, few exact results are available.[2] Thus many different approximate techniques have been developed to understand transport in disordered networks. Notable among these are computer simulations,[3] perturbation methods,[4] and the effective-medium approximation[5] (EMA) and its cluster extension.[6] The EMA is an analytical approximation that has performed well outside the critical region. In some limiting cases it is possible to obtain some information about transport properties of these networks from percolation theory using the critical-path analysis.[7] But aside from Monte Carlo methods which are purely numerical, none of the foregoing approximations is accurate in the critical region. Moreover, as the percolation threshold is approached, larger and larger networks must be used in order to maintain accuracy in the Monte Carlo approach.

Kasteleyn and Fortuin[8] showed that percolation and random conductance network problems are special cases of the q-state Potts model, so that it became possible to apply modern theory of critical phenomena to the study of percolation and conduction problems. Thus various authors have used renormalization-group methods, both in momentum[9] and in real space,[10] to study percolation and conduction near the critical point. In particular, it was shown[11] how a decimation transformation can be used to study the percolation conductivity problem near the critical point. But this method suffers from the fact that the approximations involved are extremely difficult to quantify, and it is only applicable to the critical region. Bernasconi[12] modified this method and proposed a Monte Carlo renormalization approach to the percolation conductivity problem that could handle the entire range of fraction of conducting bonds. His method yields very good results in two dimensions, but not in three dimensions (it predicts a too low bond percolation threshold and a too high conductivity critical exponent). Moreover, this method in practice is not appreciably easier to apply than the Monte Carlo method alone.

In this paper we propose a new method of approximation for the percolation conductivity problem for networks constructed on regular lattices. We combine the real-space renormalization method and EMA to obtain an approximation method, the renormalized effective-medium approximation (REMA), that is simple and yields an excellent prediction of percolation conductivity over the entire range of concentration of conducting bonds at all dimensions.

RENORMALIZED EFFECTIVE-MEDIUM APPROXIMATION

In the EMA approach,[5] the disordered network is replaced by a uniform effective medium, having the same conductance g_m between all neighboring sites. In the single-bond EMA, a single bond in the effective medium is replaced by the conductance g; the perturbation this causes in the local voltages is computed, and the value of g_m is determined by requiring that the average of the voltage perturbation equal zero when the average is computed with respect to the distribution $f(g)$ of conductances in the original disordered network. In particular, g_m is determined by the equation[5]

$$\int f(g)\frac{g-g_m}{g-(1/\gamma+1)g_m}dg=0\ . \tag{1}$$

The quantity γ is a bond Green function which depends only on the topological structure of the network and is given by $\gamma=-2/z$ for all regular networks with coordination number z. This EMA has been recently extended to hopping transport problems by several authors.[13] If the conductances are distributed according to a simple binary distribution

$$f(g)=(1-p)\delta_+(g)+p\delta(g-g_0)\ , \tag{2}$$

then the EMA predicts a bond percolation threshold $p_c = -\gamma$. In particular, it gives $\frac{1}{2}$, the exact value for the square lattice, and $\frac{1}{3}$, a value too high for the simple cubic lattice in three dimensions.

Real-space renormalization methods implement an intuitive picture proposed by Kadanoff.[14] In this picture, cells of conducting bonds in a nearly critical system behave as single bonds in a rescaled system farther from criticality. The system rescaling is achieved by removing sites and joining the remaining sites with new bonds to form a lattice of the original type. The Green function γ does not change because of rescaling since it is determined solely by the lattice topology. As was shown by Stinchcombe and Watson[11] after one rescaling from a network having the bond conductivity distribution (2) the new distribution of conductances becomes

$$\tilde{f}(g)=[1-R(p)]\delta_+(g)+\sum_{i=1}^{N} a_i(p)\delta(g-g_i)\ . \tag{3}$$

Here N is the number of possible nonzero values of g_i, the conductance of the cell that is chosen for renormalization transformation, and $a_i(p)$ is the probability that the value g_i occurs; $\sum_{i=1}^{N} a_i(p)=R(p)$, where $R(p)$ is the renormalization transformation, i.e., the probability that a bond in the rescaled network is present. In principle, one can rescale the network many times and obtain a conductivity distribution $\tilde{f}(g)$ which is a kind of "fixed-point" distribution, the shape of which does not change under further rescaling. Then the conductivity of the network can be calculated as some average of this distribution (as was done by Bernasconi[12]). However, in practice (especially in three and higher dimensions), it is very difficult to rescale the network more than once with reasonable computational effort and thus $\tilde{f}(g)$ cannot be determined exactly and one has to resort to Monte Carlo methods. It is worth mentioning that aside from one-dimensional systems, almost all renormalization transformations in two or higher dimensions are only approximate ones; exceptions are very few.[15]

It is a matter of experience that the rescaled network is farther from the critical point than the original one. Because the rescaled network is identical in topological structure to the old network, one can more accurately apply single-bond EMA to the rescaled network with $f(g)$ of Eq. (1) replaced by $\tilde{f}(g)$ as given by Eq. (3). Since the rescaled network is farther from criticality than the original network, the performance of the EMA is improved; this is the essence of our method. Because the bonds of the rescaled network are b times longer than the old one (where b is the scaling factor of the transformation), this necessitates a rescaling of conductivities for the new network to replicate the old one: The EMA conductivity for the new network is taken to be the same as that for the old one at $p=1$.

We have applied this method to bond-disordered square and simple cubic networks and the results are in good agreement with Monte Carlo simulations over the entire concentration range of the conducting bonds. Using REMA, we predict a bond percolation threshold p_c given by

$$R(p_c)=-\gamma\ . \tag{4}$$

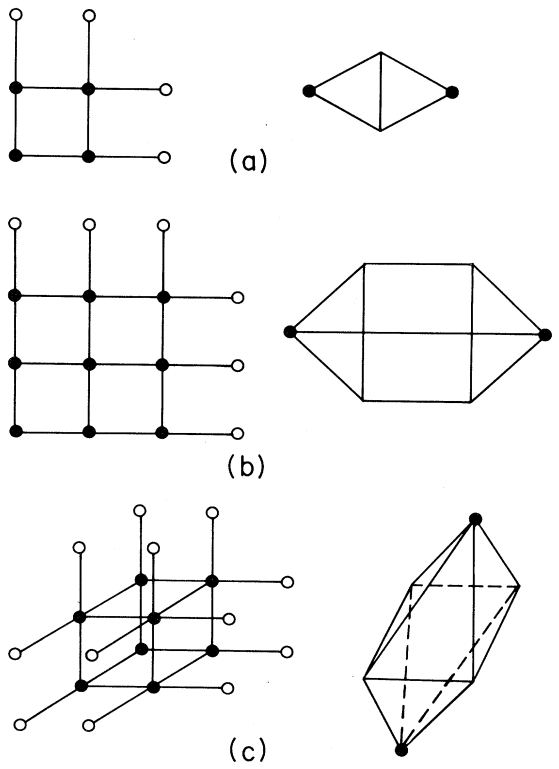

FIG. 1. Cells used for renormalizing the conductivity distribution, together with their equivalent conductance networks: (a) smallest cell for the square lattice, equivalent to a Wheatstone bridge; (b) a larger cell for the square lattice, equivalent to a generalized Wheatstone bridge; (c) cell for the simple cubic lattice, equivalent to an octahedral network.

RESULTS AND DISCUSSION

For the square lattice we used two different cells. The first one is the cell originally proposed by Reynolds *et al.*[16] [for which $b=2$, see Fig. 1(a)], and it has been used by several authors.[10] It preserves the self-duality of the square lattice and thus $p_c=\frac{1}{2}$ is the fixed point of this transformation. If we start with the binary conductance distribution (2) for individual bonds, the rescaled distribution $\tilde{f}(g)$ [the distribution of the conductance of a Wheatstone bridge as shown in Fig. 1(a)] is given by

$$\begin{aligned}\tilde{f}(g)=&[1-(p^5+5p^4q+8p^3q^2+2p^2q^3)]\delta_+(g)\\&+2p^3q^2\delta(g-\tfrac{1}{3}g_0)+2p^2(1+2p)q^2\delta(g-\tfrac{1}{2}g_0)\\&+4p^4q\delta(g-\tfrac{3}{5}g_0)+p^4\delta(g-g_0)\ .\end{aligned} \tag{5}$$

Thus

$$R(p)=p^5+5p^4q+8p^3q^2+2p^2q^3\ ,$$

where $q=1-p$ and, therefore, REMA predicts $p_c=\frac{1}{2}$. We also used a larger cell [for which $b=3$, see Fig. 1(b)]. For this cell $N=131$ and the renormalization transformation is given by

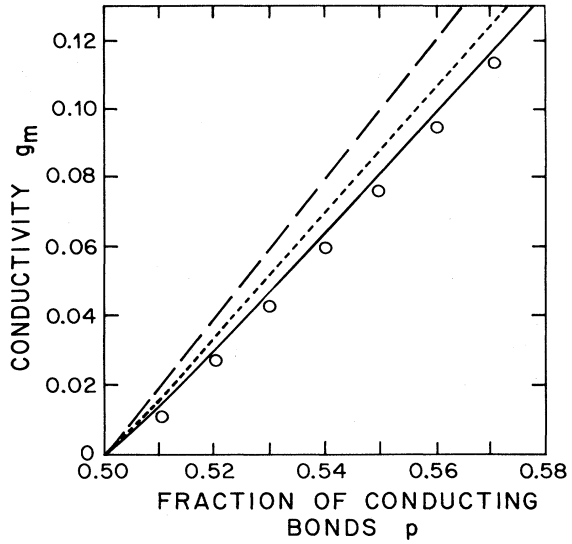

FIG. 2. Conductivity of a square lattice of random resistors in the critical region: ——, simple EMA (Ref. 5); ---, REMA ($b=2$); —, REMA ($b=3$); ○, Fogelholm's Monte Carlo data (Ref. 17).

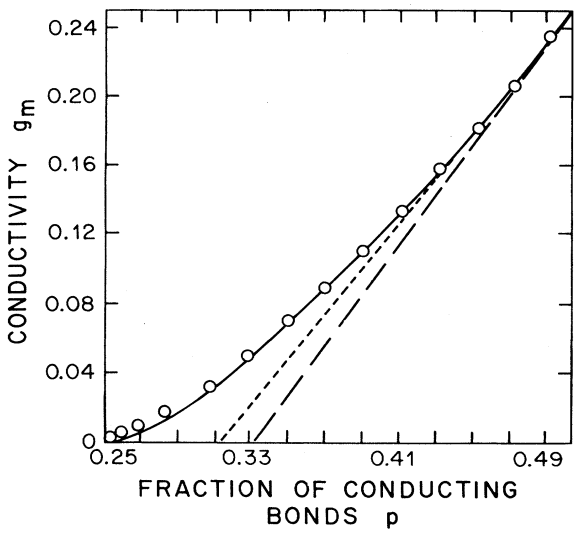

FIG. 3. Conductivity of a simple cubic lattice in the critical region: ——, simple EMA (Ref. 5); ---, cluster EMA [Ahmed and Blackman (Ref. 6)]; —, REMA; ○, Kirkpatrick's Monte Carlo data (Ref. 5).

$$R(p)=3p^3q^{10}+38p^4q^9+209p^5q^8+627p^6q^7+1089p^7q^6+1078p^8q^5+677p^9q^4+283p^{10}q^3+78p^{11}q^2+13p^{12}q+p^{13}\ . \tag{6}$$

REMA again yields $p_c=\frac{1}{2}$. In fact, Bernasconi[12] showed that this family of cells has the same self-duality as the square lattice itself. Thus $R(p_c)=\frac{1}{2}$ for all b, and since $\gamma=-\frac{1}{2}$ for the square lattice, REMA predicts $p_c=\frac{1}{2}$ for the square lattice for all b.

The conductivity of the square network in the critical region as predicted by REMA is shown in Fig. 2 where it has been compared with the data of Fogelholm[17] (the predictions of REMA outside the critical region are not shown because they are identical to Monte Carlo data of Kirkpatrick[5]). Even the predictions of REMA for $b=2$ show significant improvement over the simple EMA. It is worth mentioning that the cumulant theory of Hori and Yonezawa[4] gives poor results in two dimensions (it predicts $p_c\simeq 0.393$), whereas Bernasconi's method recovers $p_c=\frac{1}{2}$ for the square lattice.

Figure 1(c) shows the cell we used for the simple cubic calculation which was also used by Bernasconi. It is a three-dimensional version of the ($b=2$) cell that was used for square lattice. The renormalization transformation for this cell is given by

$$R(p)=p^{12}+12p^{11}q+66p^{10}q^2+220p^9q^3+493p^8q^4+776p^7q^5+856p^6q^6+616p^5q^7+238p^4q^8+48p^3q^9+4p^2q^{10}\ . \tag{7}$$

Thus REMA yields $p_c\simeq 0.265$, in agreement with the series expansion estimate[18] $p_c\simeq 0.248$, the large-cell Monte Carlo renormalization estimate[19] $p_c\simeq=0.2526$, and the conjecture of Sahimi *et al.*[20] $p_c\simeq 0.2527$. It is far superior to the $p_c\simeq 0.208$ given by Bernasconi's method, and to the $p_c=\frac{1}{3}$ which the simple EMA yields, whereas the cumulant theory[4] predicts $p_c\simeq 0.285$, a value not as impressive as the prediction of REMA.

For this cell $N=73$, i.e., there are 73 possible nonzero conductivities for the cell. The conductivity of the simple cubic lattice of random resistors in the critical region as predicted by REMA is compared with the Monte Carlo data of Kirkpatrick[5] in Fig. 3. The agreement is excellent over much of the region (the error is less than 5% for $p\geq 0.3$ and is about 7% for $0.28<p<0.3$). Also shown in Fig. 3 are the results of Ahmed and Blackman[6] who tried to improve the simple EMA by doing a cluster (consisting of 15 bonds) calculation. Their method yields $p_c\simeq 0.315$.

We point out that sufficiently close to the critical point REMA will usually predict that the conductivity goes to zero as the first power of $p-p_c$, i.e., REMA predicts that the conductivity critical exponent t equals one. This can be seen by noting that if the conductivity distribution (3) is written as

$$\tilde{f}(g)=[1-R(p)]\delta_+(g)+H(g;p)\ ,$$

then

$$g_m\int\frac{dgH(g;p)}{(1+\gamma)g_m-\gamma g}=\frac{R(p)+\gamma}{1+\gamma}\ , \tag{8}$$

so that as long as $H_{-1}(p)$ and $H_{-2}(p)$ are finite (see Sahimi *et al.*[13]), where

$$H_{-n}(p)=\int H(g;p)g^{-n}dg$$

(as will be the case if the original distribution is binary and the renormalizing cell is of finite size), the asymptotic behavior of the predicted conductivity is

$$g_m=\alpha(p-p_c)+\beta(p-p_c)^2+o((p-p_c)^2)\ , \tag{9}$$

where

$$\alpha=\frac{|\gamma|R'(p_c)}{H_{-1}(p_c)(1+\gamma)} \tag{10}$$

and

$$\beta=\frac{(1+\gamma)H_{-2}(p_c)}{|\gamma|H_{-1}(p_c)}\alpha^2-\frac{H'_{-1}(p_c)}{H_{-1}(p_c)}\alpha+\frac{|\gamma|R''(p_c)}{2(1+\gamma)H_{-1}(p_c)} . \tag{11}$$

REMA therefore appears to fail in the critical region, since it is believed[1] that $t>1$. However, even for small renormalizing cells, this linear region is quite small compared to the physical critical region (by which we mean the region where the conductivity has distinct curvature). A quantitative estimate of the width of the linear region can be made from Eq. (9) by finding those values of $p-p_c$ for which the second term of the REMA conductivity fails to exceed a fraction k of the first term, viz.,

$$p-p_c \le W(k)\equiv k\,|\alpha/\beta| . \tag{12}$$

For example, for the square lattice with the smallest cell ($b=2$), we find that $p-p_c \le 0.2k$ estimates the linear region. Taking k as large as 0.1, we find that $p-p_c \le 0.02$, a very small region. Thus it is possible to use REMA to estimate the true exponent by analysis of the conductivity curve just outside $p-p_c \le W(k)$. For the square lattice we analyzed the predictions of REMA (for $b=3$) outside $p-p_c<0.02$ up to $p-p_c=0.1$. This yielded $t=1.12\pm0.05$. The value of t has been reported by several authors and has been found to be anywhere from[21] $t=1$ to[22] $t=1.43$ (For a review see Sahimi.[23]) Our finding is consistent with Kirkpatrick's[5] who found $1<t<1.3$ and with Straley's[3] who obtained $t=1.1\pm0.05$ for the square network. However, very recently Derrida and Vannimenus[24] applied a transfer-matrix method (which is believed to be very accurate) to random conductance networks and obtained $t=1.28\pm0.03$, which is consistent with Fogelholm's[17] finding $t=1.31\pm0.04$, whose data are compared with REMA predictions. Thus it appears that the REMA prediction of t in two dimensions is somewhat low, but a larger cell, e.g., $b=4$, will definitely improve the prediction.

For the cubic network we analyzed the predictions of REMA in the range $0.28<p<0.45$. This yielded $t=1.55\pm0.1$. This is definitely consistent with Kirkpatrick's[5] $t=1.6\pm0.1$ (bond) and $t=1.5\pm0.2$ (site), with $t=1.6\pm0.1$ (bond) of Webman *et al.*,[3] and with Straley's[3] $t=1.7\pm0.1$ (bond), whereas Bernasconi obtained $t=2.14\pm0.02$, which seems to be rather high. This is because in his method p_c is too low and thus the renormalization transformation overestimates the length of the critical region; thus the value of t predicted is too high. We note, however, that our estimate of t is lower than the prediction of the finite-size scaling method[25] $t=1.87\pm0.04$ as is expected.

We consider now a random conductance network for which the individual bond conductances have the distribution

$$f(g)=(1-p)\delta(g-g_0)+p\delta(g-\infty) , \tag{13}$$

i.e., if a fraction $(1-p)$ of bonds are ordinary conductors and the remaining fractions p of them are superconducting. For $p>p_c$ the network is superconducting. The conductivity g_m of the network diverges as the percolation threshold is approached from below (i.e., as the perfect metallic state is approached), with a power law dependence of the form

$$g_m \sim (p_c-p)^{-s} . \tag{14}$$

In two dimensions a simple application of the duality transformation by Straley[3] shows that $s=t$. REMA satisfies this duality relation, as does the simple EMA (as was shown by Bernasconi *et al.*[2]). For the simple cubic network in three dimensions we obtained $s=0.89+0.09$. This should be compared with Straley's[3] estimate $s=0.7\pm0.05$ and with the estimate $s=0.9\pm0.1$ of Webman *et al.*[26] Simple EMA yields $s=1$, while Bernasconi obtained $s=0.76\pm0.01$. We finally remark that REMA predicts the exact slopes of $g_m(p)$ at $p=1$ and $p=0$ in two dimensions as does the simple EMA.

SUMMARY AND CONCLUSIONS

We have developed a new method of predicting the percolation conductivity by combining real-space renormalization and EMA methods. Very good agreement is found between REMA predictions and those of Monte Carlo data in two dimensions; in three dimensions the predictions are excellent. The ideas presented in this paper can be used to calculate t and p_c very accurately in dimensions higher than three. For example a four-dimensional version of the cell that was used in three dimensions[19] yields $p_c=0.157$ with REMA, in excellent agreement with the series expansion estimate[27] $p_c=0.161$ and the conjecture of Sahimi *et al.*[20] $p_c=0.156$. Simple EMA yields $p_c=0.25$ for $d=4$. These ideas can also be modified for percolation conductivity problems in other d-dimensional cubic networks and in site-disordered random resistor networks. The results will be reported elsewhere in a planned future publication.

ACKNOWLEDGMENT

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