Journal of Statistical Physics, Vol. 108, Nos. 5/6, September 2002 (© 2002)

On Effective Conductivity on $\mathbb{Z}^d$ Lattice

Leonid G. Fel[1] **and Konstantin M. Khanin**[2]

Received November 29, 2001; accepted April 10, 2002

We study the effective conductivity σ_e for a random wire problem on the d-dimensional cubic lattice $\mathbb{Z}^d$, $d \geqslant 2$ in the case when random conductivities on bonds are independent identically distributed random variables. We give exact expressions for the expansion of the effective conductivity in terms of the moments of the disorder parameter up to the 5th order. In the 2D case using the duality symmetry we also derive the 6th order expansion. We compare our results with the Bruggeman approximation and show that in the 2D case it coincides with the exact solution up to the terms of 4th order but deviates from it for the higher order terms.

KEY WORDS: Effective conductivity; Bruggeman's equation.

1. INTRODUCTION

The problem of conductivity of the random composite medium and the equivalent problem of diffusion in a symmetric (self-adjoint) random environment has been a subject of intensive study for the last 25 years. It is virtually impossible to give a full reference list and we just mention few papers where the mathematical aspects of the theory were considered for the first time: refs. 1–4. In the mathematical literature this problem usually is quoted as the problem of homogenization for the second order elliptic differential operators with random coefficients. Roughly speaking the main result can be formulated in the following way: there exists a non-random effective conductivity tensor or effective diffusion matrix such that the asymptotic properties of the system are the same as for a homogeneous

Dedicated to D. Ruelle and Ya. G. Sinai on occasion of their 65th birthday.

[1] School of Physics and Astronomy of Exact Sciences, Tel Aviv University, Ramat Aviv 69978, Israel.

[2] Isaac Newton Institute for Mathematical Sciences, University of Cambridge, 20 Clarkson Road, Cambridge CB3 OEH, United Kingdom; e-mail: kk262@newton.cam.ac.uk

system governed by the effective parameters. The subject is a very active research area till now with a vast number of papers publishing every year. However there are very few results related to the problem of calculation of effective conductivity and diffusion matrix. In addition to the trivial one-dimensional case such results are known only in the self-dual situation in dimension two (Keller–Dykhne duality) and in the case of two-component systems where the analytic continuation method is used to express the effective conductivity as an analytic function of the ratio of the conductivities of two components (see refs. 5–9). In this paper we discuss a very general rigorous method in the lattice case which was developed in ref. 4. The method is based on a convergent power series expansion for the effective parameters and can be applied for arbitrary probability distribution of random conductivities. However, the combinatorics of this expansion is rather complicated. That is a reason why it was not used for concrete calculations in the past.

The present paper has two main goals. First of all we demonstrate the constructive potential of the method in ref. 4 and give exact formulae for the first 5 orders of the expansion for the effective conductivity in arbitrary dimension. In the 2D case we also calculate the 6th order terms. We then use our exact results to study the quality of the classical Bruggeman approximation. We show that in the 2D case the Bruggeman approximation is extremely accurate and coincides with the exact answer up to the terms of the 4th order. We assume everywhere that the random conductivities (jump rates) are independent identically distributed random variables. Although we consider only the case of $\mathbb{Z}^d$ lattice we strongly believe that the method can be generalized for other types of lattices and even for the continuous situation.

Yakov Sinai was a teacher of one of us and it is our pleasure to dedicate this paper to his 65th birthday. In fact one of the motivations for this paper was to illuminate the method developed together with Yakov Grigorevich and to demonstrate its effective power.

2. EFFECTIVE CONDUCTIVITY ON $\mathbb{Z}^d$ LATTICE

2.1. Exact Expansion for Effective Conductivity

We consider effective conductivity for a random wire problem on the d-dimensional cubic lattice $\mathbb{Z}^d$, $d \geqslant 2$. Throughout the paper we assume that bond conductivities σ are independent identically distributed positive random variables. We are not making any assumptions on a probability distribution of σ which can be either discrete or continuous. As we have mentioned above the calculation of the effective conductivity is equivalent to the calculation of the effective diffusion matrix for the continuous time random walk in random environment. In this case random conductivities should be understood as jump rates through the corresponding bond. We shall use the formula for the effective diffusion matrix M_e which was obtained in ref. 4. This formula is given by a convergent series where the role of small parameter is played by a deviation of a random variable σ from its average value $\langle\sigma\rangle$. Since we consider transitions only along the bonds of $\mathbb{Z}^d$ lattice with i.i.d. transition rates σ, the effective diffusion matrix is a scalar matrix: $M_e = 2\sigma_e I$, where effective diffusion coefficient (or effective conductivity) σ_e can be expressed in terms of a convergent power series. We first introduce the necessary notations.

A path $\gamma = \{(z_1, \alpha_1), (z_2, \alpha_2),..., (z_k, \alpha_k)\}$ is a finite sequence of pairs (z, α) where z is a point of lattice $\mathbb{Z}^d$ and $\alpha = 1, 2,..., d$ corresponds to one of the d possible directions. Notice that z_i, z_{i+1} are not necessarily neighbours on the lattice. The sum of two paths $\gamma = \gamma_1 + \gamma_2$ is simply the ordered union of two sequences where the pairs of the second path follow the pairs of the first one. With each pair (z, α) we associate a random variable $\sigma_\alpha(z) = \sigma(z, z+e_\alpha)$, where e_α is a unit vector in the direction α and $\sigma(z, z+e_\alpha)$ is the random transition rate (conductivity) along the bond $(z, z+e_\alpha)$. Denote by $u_\alpha(z) = \frac{\sigma_\alpha(z) - \langle\sigma\rangle}{\langle\sigma\rangle}$ and define for each path $\gamma = \{(z_1, \alpha_1), (z_2, \alpha_2),..., (z_k, \alpha_k)\}$ the moment

$$\langle\gamma\rangle = \left\langle \prod_{i=1}^{k} u_{\alpha_i}(z_i) \right\rangle. \tag{1}$$

A convergent expansion below for the effective conductivity is expressed through the moments of a random variable u. We shall also need the following cumulant of a path γ:

$$E(\gamma) = \sum_{m=1}^{k} (-1)^{m-1} \sum_{\gamma_1 + \cdots + \gamma_m = \gamma} \prod_{j=1}^{m} \langle\gamma_j\rangle, \tag{2}$$

where summation in (2) is taken over all possible partitions of the path γ into a sum of paths γ_j. Finally we define a kernel $\Gamma_{\alpha\beta}(z)$:

$$\Gamma_{\alpha\beta}(z) = -\int_0^1 \cdots \int_0^1 \frac{\sin \pi\lambda_\alpha \sin \pi\lambda_\beta \cos 2\pi((\lambda, z) - \frac{1}{2}\lambda_\alpha + \frac{1}{2}\lambda_\beta)}{\sum_{\gamma=1}^{d} \sin^2 \pi\lambda_\gamma} \prod_{\gamma=1}^{d} d\lambda_\gamma, \tag{3}$$

where $\lambda = (\lambda_1,..., \lambda_d)$. Notice that $\Gamma_{\alpha\alpha}(0) = -\frac{1}{d}$ and $\Gamma_{\alpha\beta}(z) = \Gamma_{\beta\alpha}(-z)$. We can now write the following exact formula for σ_e:

$$\sigma_e = \langle\sigma\rangle\left(1 + \sum_{k=2}^{\infty} A^{(k)}\right), \tag{4}$$

where

$$A^{(k)} = \sum_{\gamma = \{(z_1, \alpha_1),\dots, (z_k, \alpha_k)\} \in \mathscr{G}_1^{(k)}} E(\gamma) \prod_{i=1}^{k-1} \Gamma_{\alpha_i \alpha_{i+1}}(z_{i+1} - z_i). \tag{5}$$

Here $\mathscr{G}_1^{(k)}$ is the set of all possible paths $\gamma = \{(z_1, \alpha_1),\dots, (z_k, \alpha_k)\}$ such that $z_1 = 0$ and $\alpha_1 = \alpha_d = 1$. It has been proven in ref. 4 that the infinite sum in (5) is absolutely convergent. That is due to the fact that for the paths γ which might lead to divergence of $A^{(k)}$ one has $E(\gamma) = 0$. It was also shown that the expansion in (4) is absolutely convergent and gives an exact value of σ_e provided $|u| \leqslant u_0 < 1/2$. The last condition is technical and probably can be improved. In the following proposition we rewrite (4), (5) in a slightly different way.

Proposition 1 (ref. 4). Assume that there exists a constant $u_0 < \frac{1}{2}$ such that $|u| \leqslant u_0$ with probability 1. Then for any dimension d

$$\sigma_e = \langle \sigma \rangle \left(1 + \sum_{k=2}^{\infty} \sum_{m=1}^{[\frac{k}{2}]} \sum_{\substack{s_1,\dots, s_m \geqslant 2 \\ s_1 + \cdots + s_m = k}} a^d_{s_1,\dots, s_m} \langle u^{s_1} \rangle \cdots \langle u^{s_m} \rangle \right), \tag{6}$$

where the constants $a^d_{s_1,\dots, s_m}$ depend only on dimension d and $[\,\cdot\,]$ denotes the integer part. Moreover, for any $n \geqslant 1$ the following estimate holds

$$\left| \sigma_e - \langle \sigma \rangle \left(1 + \sum_{k=2}^{n} \sum_{m=1}^{[\frac{k}{2}]} \sum_{\substack{s_1,\dots, s_m \geqslant 2 \\ s_1 + \cdots + s_m = k}} a^d_{s_1,\dots, s_m} \langle u^{s_1} \rangle \cdots \langle u^{s_m} \rangle \right) \right| \leqslant \frac{(2u_0)^{n+1}}{1 - 2u_0}. \tag{7}$$

Note that the series in (6) is absolutely convergent.

2.2. The 4th Order Expansion

It is easy to see that only those paths for which each pair (z, α) is present at least twice give nonzero contribution to (5). This immediately implies that

$$A^{(2)} = \langle u^2 \rangle\, \Gamma_{11}(0) = -\frac{\langle u^2 \rangle}{d}, \qquad A^{(3)} = \langle u^3 \rangle\, \Gamma_{11}^2(0) = \frac{\langle u^3 \rangle}{d^2}. \tag{8}$$

Hence the 3rd order approximation to σ_e is given by

$$\sigma_e^{(3)} = \langle \sigma \rangle \left(1 - \frac{\langle u^2 \rangle}{d} + \frac{\langle u^3 \rangle}{d^2} \right). \tag{9}$$

In the 4th order the combinatorics is slightly more complicated. Indeed, nonzero contributions correspond to the paths

$$\begin{aligned}
\gamma(4) &= \{(0,1),(0,1),(0,1),(0,1)\}, \\
\gamma^1_{1,z}(4) &= \{(0,1),(z,1),(z,1),(0,1)\}, \qquad z\neq 0, \\
\gamma_{\alpha,z}(4) &= \{(0,1),(z,\alpha),(z,\alpha),(0,1)\}, \qquad \alpha\neq 1, \\
\gamma^2_{1,z}(4) &= \{(0,1),(z,1),(0,1),(z,1)\}, \qquad z\neq 0.
\end{aligned}$$

Another possible type of paths $\gamma^3_{1,z}(4)=\{(0,1),(0,1),(z,1),(z,1)\}$, $z\neq 0$ gives zero contribution since $E(\gamma^3_{1,z}(4))=0$. Easy calculation gives

$$\begin{aligned}
A^{(4)} &= [(\langle u^4\rangle-\langle u^2\rangle^2)\,\Gamma^3_{11}(0)]+\left[\langle u^2\rangle^2\,\Gamma_{11}(0)\Big(\sum_{z\in\mathbb{Z}^d}\Gamma^2_{11}(z)-\Gamma^2_{11}(0)\Big)\right] \\
&\quad+\left[\langle u^2\rangle^2\Big(\sum_{z\in\mathbb{Z}^d}\Gamma^3_{11}(z)-\Gamma^3_{11}(0)\Big)\right]+\sum_{\alpha=2}^{d}\left[\langle u^2\rangle^2\,\Gamma_{\alpha\alpha}(0)\sum_{z\in\mathbb{Z}^d}\Gamma^2_{1\alpha}(z)\right].
\end{aligned} \tag{10}$$

Notice that

$$\sum_{z\in\mathbb{Z}^d}\Gamma^2_{\beta\alpha}(z)=\int_0^1\cdots\int_0^1\frac{\sin^2\pi\lambda_\beta\,\sin^2\pi\lambda_\alpha}{(\sum_{\gamma=1}^d\sin^2\pi\lambda_\gamma)^2}\prod_{\gamma=1}^d d\lambda_\gamma. \tag{11}$$

Hence

$$\sum_{\beta,\alpha=1}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma^2_{\beta\alpha}(z)=1. \tag{12}$$

Since

$$\sum_{\alpha=1}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma^2_{\beta\alpha}(z) \tag{13}$$

does not depend on β we get

$$\sum_{\alpha=1}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma^2_{1\alpha}(z)=\frac{1}{d}. \tag{14}$$

Using (10, 14) we obtain

$$A^{(4)}=-\frac{1}{d^3}\langle u^4\rangle-\frac{d-2}{d^3}\langle u^2\rangle^2+\langle u^2\rangle^2\sum_{z\neq 0}\Gamma^3_{11}(z). \tag{15}$$

The third term in (15) vanishes in the 2D case. Indeed, if $z=(x, y)$ we have $\Gamma_{11}(x, y)=\Gamma_{22}(y, x)$. Obviously $\Gamma_{11}(y, x)+\Gamma_{22}(y, x)=0$ if $(y, x)\neq(0, 0)$. Hence, for nonzero (x, y) we have $\Gamma_{11}(y, x)=-\Gamma_{11}(x, y)$ which immediately implies $\sum_{z\neq 0}\Gamma^3_{11}(z)=0$. As a result we obtain the 4th order approximation for $d=2$:

$$\sigma_e^{(4)}=\langle\sigma\rangle(1-\tfrac{1}{2}\langle u^2\rangle+\tfrac{1}{4}\langle u^3\rangle-\tfrac{1}{8}\langle u^4\rangle). \tag{16}$$

We next demonstrate that for $d\geqslant 3$

$$\sum_{z\in\mathbb{Z}^d}\Gamma^3_{11}(z)\neq-\frac{1}{d^3} \tag{17}$$

which implies

$$\sum_{z\neq 0}\Gamma^3_{11}(z)\neq 0. \tag{18}$$

Denote $H(d)=-d^3\sum_{z\in\mathbb{Z}^d}\Gamma^3_{11}(z)$. Using simple Fourier analysis we have

$$H(d)=\int_0^1\cdots\int_0^1 H(\lambda, \mu)\prod_{\gamma=1}^d d\lambda_\gamma\prod_{\gamma=1}^d d\mu_\gamma, \tag{19}$$

where

$$H(\lambda, \mu)=\frac{\sin^2(\pi(\lambda_1+\mu_1))}{\frac{1}{d}\sum_{\gamma=1}^d\sin^2(\pi(\lambda_\gamma+\mu_\gamma))}\frac{\sin^2(\pi\lambda_1)}{\frac{1}{d}\sum_{\gamma=1}^d\sin^2(\pi\lambda_\gamma)}\frac{\sin^2(\pi\mu_1)}{\frac{1}{d}\sum_{\gamma=1}^d\sin^2(\pi\mu_\gamma)}. \tag{20}$$

As we have explained above the symmetry in the 2D case gives $\sum_{z\neq 0}\Gamma^3_{11}(z)=0$ which is equivalent to $H(2)=1$. We conjecture that $H(d)$ is a strictly decreasing function of d. The conjecture implies that $\sum_{z\neq 0}\Gamma^3_{11}(z)>0$ for all $d\geqslant 3$. Although the conjecture above was not proven rigorously we have checked it numerically for $3\leqslant d\leqslant 5$:

$$H(3)=0.923,\qquad H(4)=0.874,\qquad H(5)=0.846. \tag{21}$$

Finally, we get the following 4th order approximation in an arbitrary dimension:

$$\sigma_e^{(4)}=\langle\sigma\rangle\left(1-\frac{1}{d}\langle u^2\rangle+\frac{1}{d^2}\langle u^3\rangle-\frac{1}{d^3}\langle u^4\rangle-\frac{d+H(d)-3}{d^3}\langle u^2\rangle^2\right). \tag{22}$$

2.3. The 5th Order Expansion

We proceed with the 5th order calculations. The following paths give nonzero contributions:

$$\gamma(5) = \{(0,1),(0,1),(0,1),(0,1),(0,1)\},$$

$$\gamma^1_{\alpha,z}(5) = \{(0,1),(z,\alpha),(z,\alpha),(z,\alpha),(0,1)\}$$

$$\gamma^2_{\alpha,z}(5) = \{(0,1),(0,1),(z,\alpha),(z,\alpha),(0,1)\},$$

$$\gamma^3_{\alpha,z}(5) = \{(0,1),(z,\alpha),(0,1),(z,\alpha),(0,1)\}$$

$$\gamma^4_{\alpha,z}(5) = \{(0,1),(z,\alpha),(z,\alpha),(0,1),(0,1)\},$$

$$\tilde{\gamma}^1_{1,z}(5) = \{(0,1),(z,1),(0,1),(z,1),(z,1)\}$$

$$\tilde{\gamma}^2_{1,z}(5) = \{(0,1),(z,1),(z,1),(0,1),(z,1)\},$$

$$\tilde{\gamma}^3_{1,z}(5) = \{(0,1),(z,1),(0,1),(0,1),(z,1)\}$$

$$\tilde{\gamma}^4_{1,z}(5) = \{(0,1),(0,1),(z,1),(0,1),(z,1)\}.$$

Notice that in the case $\alpha = 1$ the summation in the paths $\gamma^s_{1,z}(5)$, $\tilde{\gamma}^s_{1,z}(5)$, $1 \leqslant s \leqslant 4$ is performed over all $z \neq 0$. Using (5) we get

$$A^{(5)} = \frac{1}{d^4}\langle u^5\rangle + K_5(d)\langle u^2\rangle\langle u^3\rangle, \tag{23}$$

where

$$K_5(d) = \sum_{\alpha=1}^{d}\left(\frac{3}{d^2}\sum_{z\in\mathbb{Z}^d}\Gamma^2_{1\alpha}(z) + \sum_{z\in\mathbb{Z}^d}\Gamma^4_{1\alpha}(z)\right) - \frac{6}{d^4} - \frac{4}{d}\sum_{z\neq 0}\Gamma^3_{11}(z). \tag{24}$$

This together with (14) gives

$$K_5(d) = \frac{3(d-2)}{d^4} + \sum_{\alpha=1}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma^4_{1\alpha}(z) - \frac{4}{d}\sum_{z\neq 0}\Gamma^3_{11}(z). \tag{25}$$

In the 2D case both the first and the last term in (25) vanish and

$$K_5(2) = \sum_{z\in\mathbb{Z}^2}\Gamma^4_{11}(z) + \sum_{z\in\mathbb{Z}^2}\Gamma^4_{12}(z) = I_1 + I_2, \tag{26}$$

where

$$I_1=\int_0^1\int_0^1 h_1^2(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2,$$
$$h_1(\lambda_1,\lambda_2)=\int_0^1\int_0^1 \frac{\sin^2\pi(\lambda_1-\mu_1)\sin^2\pi\mu_1\,d\mu_1\,d\mu_2}{(\sin^2\pi(\lambda_1-\mu_1)+\sin^2\pi(\lambda_2-\mu_2))(\sin^2\pi\mu_1+\sin^2\pi\mu_2)} \tag{27}$$

and

$$I_2=\int_0^1\int_0^1 h_2^2(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2,$$
$$h_2(\lambda_1,\lambda_2)=\int_0^1\int_0^1 \frac{\sin\pi(\lambda_1-\mu_1)\sin\pi(\lambda_2-\mu_2)\sin\pi\mu_1\sin\pi\mu_2\,d\mu_1\,d\mu_2}{(\sin^2\pi(\lambda_1-\mu_1)+\sin^2\pi(\lambda_2-\mu_2))(\sin^2\pi\mu_1+\sin^2\pi\mu_2)}. \tag{28}$$

The values of I_1, I_2 were found numerically: $I_1=0.06391$, $I_2=0.00439$. As a result we get in the 2D case the following 5th order expansion:

$$\sigma_e^{(5)}=\langle\sigma\rangle(1-\tfrac{1}{2}\langle u^2\rangle+\tfrac{1}{4}\langle u^3\rangle-\tfrac{1}{8}\langle u^4\rangle+\tfrac{1}{16}\langle u^5\rangle+I\langle u^2\rangle\langle u^3\rangle), \tag{29}$$

where $I=I_1+I_2=0.0683$.

In the general case $d\geqslant 3$ we have

$$\sum_{\alpha=1}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma_{1\alpha}^4(z)=\sum_{z\in\mathbb{Z}^d}\Gamma_{11}^4(z)+\sum_{\alpha=2}^{d}\sum_{z\in\mathbb{Z}^d}\Gamma_{1\alpha}^4(z)=I_1(d)+(d-1)\,I_2(d), \tag{30}$$

where

$$I_1(d)=\int_0^1\cdots\int_0^1 h_1^2(\lambda)\prod_{\gamma=1}^{d}d\lambda_\gamma,$$
$$h_1(\lambda)=\int_0^1\cdots\int_0^1 \frac{\sin^2\pi(\lambda_1-\mu_1)\sin^2\pi\mu_1\prod_{\gamma=1}^{d}d\mu_\gamma}{(\sum_{\gamma=1}^{d}\sin^2(\pi(\lambda_\gamma-\mu_\gamma)))(\sum_{\gamma=1}^{d}\sin^2(\pi\mu_\gamma))} \tag{31}$$

and

$$I_2(d)=\int_0^1\cdots\int_0^1 h_2^2(\lambda)\prod_{\gamma=1}^{d}d\lambda_\gamma,$$
$$h_2(\lambda)=\int_0^1\cdots\int_0^1 \frac{\sin\pi(\lambda_1-\mu_1)\sin\pi(\lambda_2-\mu_2)\sin\pi\mu_1\sin\pi\mu_2\prod_{\gamma=1}^{d}d\mu_\gamma}{(\sum_{\gamma=1}^{d}\sin^2(\pi(\lambda_\gamma-\mu_\gamma)))(\sum_{\gamma=1}^{d}\sin^2(\pi\mu_\gamma))}. \tag{32}$$

Collecting all the terms we get

$$\sigma_e^{(5)} = \langle\sigma\rangle\Bigg(1-\frac{1}{d}\langle u^2\rangle+\frac{1}{d^2}\langle u^3\rangle-\frac{1}{d^3}\langle u^4\rangle-\frac{d+H(d)-3}{d^3}\langle u^2\rangle^2 \\ +\frac{1}{d^4}\langle u^5\rangle+\frac{3d+d^4I(d)+4H(d)-10}{d^4}\langle u^2\rangle\langle u^3\rangle\Bigg), \tag{33}$$

where $I(d)=I_1(d)+(d-1)\,I_2(d)$ and $H(d)$ is given by (19), (20).

2.4. Keller–Dykhne Duality and the 6th Order Expansion in the 2D Case

Although it is possible in principle to calculate an expansion of an arbitrary order the problem becomes more and more cumbersome for higher order terms. However in the 2D case one can significantly simplify calculations using the duality symmetry which was discovered by Keller[10] and Dykhne.[11] Consider duality transformation

$$\sigma \to \frac{1}{\sigma}. \tag{34}$$

Denote by $\{\sigma\}$, $\{\sigma^{-1}\}$ the probability distributions for positive random variables σ and σ^{-1} respectively. Then duality symmetry which holds only in the 2D case implies that

$$\sigma_e(\{\sigma^{-1}\})=\sigma_e^{-1}(\{\sigma\}). \tag{35}$$

Although both Keller and Dykhne considered only the continuous systems the symmetry (35) can be extended to the case of discrete lattice systems which we study in this paper (see ref. 12). The duality symmetry immediately implies that in the self-dual case, i.e., when the probability distributions $\{\sigma\}$ and $\{\sigma^{-1}\}$ coincide, the effective conductivity $\sigma_e=1$. It also gives an exact answer in the case which we call almost self-dual. We say that the probability distribution for a random variable σ is almost self-dual with respect to the duality transformation (34) if there exists a positive constant σ_0 such that the probability distribution for $\sigma_0\sigma$ is exactly self-dual, i.e.,

$$\{\sigma_0\sigma\}=\{(\sigma_0\sigma)^{-1}\}. \tag{36}$$

Since σ_e is a homogeneous function of the first order and $\sigma_e(\{\sigma_0\sigma\})=1$, it follows that in the almost self-dual situation $\sigma_e(\{\sigma\})=\sigma_0^{-1}$. Notice that in the two-component case with equipartition, i.e., when σ takes values σ_1 and σ_2 with probabilities $\frac{1}{2}$ the probability distribution for σ is almost self-dual with $\sigma_0=(\sqrt{\sigma_1\sigma_2})^{-1}$. Hence,

$$\sigma_e=\sigma_0^{-1}=\sqrt{\sigma_1\sigma_2}. \tag{37}$$

This well-known result by Keller and Dykhne provides one of the very few exact solutions for the effective conductivity.

We next show that the duality symmetry alone gives a lot of relations on the coefficients of the expansion (6). In fact we shall be able to recover the 6th order expansion using only the 5th order and the symmetry. Consider the case when σ takes three values: $1-\epsilon$ with probability p, $1-\alpha\epsilon$ with probability p and 1 with probability $1-2p$. Correspondingly a random variable σ^{-1} takes values $\frac{1}{1-\epsilon}$ and $\frac{1}{1-\alpha\epsilon}$ with probabilities p and 1 with probability $1-2p$. We shall use the formula (6) in order to calculate $\sigma_e(\{\sigma\})\,\sigma_e(\{\sigma^{-1}\})$ and check the duality identity (35) subsequently in the 2nd, 4th, 6th and 8th orders of the power series expansion in ϵ. This inductive procedure allows to find all the relations on the coefficients $a^2_{s_1,\dots,s_m}$. We performed calculations using the Maple symbolic package. In the 2nd order one immediately gets $a^2_2=-\frac{1}{2}$. The 4th order calculations give two relations:

$$a^2_{2,2}=\tfrac{3}{2}a^2_3-\tfrac{3}{8},\qquad a^2_4=\tfrac{1}{4}-\tfrac{3}{2}a^2_3. \tag{38}$$

The 6th order expansion provides four more relations:

$$\begin{aligned} a^2_{2,2,2}&=\tfrac{7}{2}a^2_3+\tfrac{3}{2}a^2_{2,3}-\tfrac{15}{16}, & a^2_{3,3}&=\tfrac{1}{2}+\tfrac{1}{2}(a^2_3)^2-2a^2_3-a^2_{2,3},\\ a^2_{2,4}&=\tfrac{11}{8}-6a^2_3-\tfrac{3}{2}a^2_{2,3}+\tfrac{5}{2}a^2_5, & a^2_6&=\tfrac{5}{2}a^2_3-\tfrac{5}{2}a^2_5-\tfrac{1}{2}. \end{aligned} \tag{39}$$

Using (29) we have

$$a^2_3=\tfrac{1}{4},\qquad a^2_5=\tfrac{1}{16},\qquad a^2_{2,3}=I=0.0683 \tag{40}$$

which immediately gives $a^2_{2,2}=0$, $a^2_4=-\frac{1}{8}$ and

$$a^2_{2,2,2}=\tfrac{3}{2}I-\tfrac{1}{16},\qquad a^2_{3,3}=\tfrac{1}{32}-I,\qquad a^2_{2,4}=\tfrac{1}{32}-\tfrac{3}{2}I,\qquad a^2_6=-\tfrac{1}{32}. \tag{41}$$

As a result we obtain the 6th order expansion in the 2D case:

$$\begin{aligned}\sigma_e^{(6)}=\langle\sigma\rangle\big(1&-\tfrac{1}{2}\langle u^2\rangle+\tfrac{1}{4}\langle u^3\rangle-\tfrac{1}{8}\langle u^4\rangle+\tfrac{1}{16}\langle u^5\rangle+I\langle u^2\rangle\langle u^3\rangle\\ &-\tfrac{1}{32}\langle u^6\rangle-(\tfrac{3}{2}I-\tfrac{1}{32})\langle u^2\rangle\langle u^4\rangle-(I-\tfrac{1}{32})\langle u^3\rangle^2+(\tfrac{3}{2}I-\tfrac{1}{16})\langle u^2\rangle^3\big).\end{aligned} \tag{42}$$

3. THE BRUGGEMAN APPROXIMATION

3.1. Bruggeman's Equation

The Effective Medium Approximation (EMA) was invented by Bruggeman,[13] and has remained one of the most popular approximations used for calculations of the linear bulk effective electrical conductivity σ_e of a many-component composite medium. This is mainly due to the simplicity of EMA and to the fact that it gives accurate results for a wide range of parameters. It also has a non-trivial percolation threshold which most other simple approximations do not possess. Another advantage of Bruggeman's approximation is connected with the fact that none of the complicated details of the microstructure are used in its construction. EMA is only based on the assumptions that the composite is macroscopically homogeneous and isotropic and that individual grains are spherical. It is also important to mention that EMA applies without any changes to the calculation of dielectric susceptibility, magnetic permeability, thermal conductivity and chemical diffusion coefficients, since in all those cases the mathematical structure of the equations is the same as for electrical conduction.

Suppose that the values of the component conductivities σ_i and the component volume fractions p_i are given. Then Bruggeman's equation in the d-dimensional case has the following form:

$$\sum_{i=1}^{n} p_i \, \frac{\sigma_i - \sigma_B}{\sigma_i + (d-1)\, \sigma_B} = 0\,. \tag{43}$$

From the mathematical standpoint it has many beautiful properties which are of high importance for the theory of random composites. Equation (43) has a unique positive root $\sigma_B(\sigma_i)$ which is homogeneous of the first order, monotone and reducible with respect to the equating of some constituents. It is also S_n-permutation invariant in the case when all p_i are equal and compatible with a trivial solution $\sigma_B = \bar{\sigma}$ when all $\sigma_i = \bar{\sigma}$. Finally, in the case $d = 2$ the Bruggeman's solution is self-dual with respect to the duality transformation (34). Namely, if $\sigma_i \to \sigma_i^{-1}$ and p_i are unchanged then

$$\sigma_B(\sigma_1^{-1}, \sigma_2^{-1}, \ldots, \sigma_n^{-1}) = \sigma_B^{-1}(\sigma_1, \sigma_2, \ldots, \sigma_n)\,. \tag{44}$$

It follows that σ_B coincides with Keller–Dykhne solutions in the self-dual and almost self-dual situations. In particular, $\sigma_B = \sqrt{\sigma_1 \sigma_2}$ for the two-component system with equipartition and conductivities taken values σ_1, σ_2. Notice that the Bruggeman approximation is also exact in the 1D case.

3.2. Solution of Bruggeman's Equation

Let σ be a random variable corresponding to random conductivity. Then Bruggeman's equation (43) can be written in terms of averages in the following form

$$\left\langle \frac{\sigma-\sigma_B}{\sigma+(d-1)\,\sigma_B} \right\rangle = 0. \tag{45}$$

Notice that (45) is the most general form of Bruggeman's equation. We first show that Bruggeman's equation (45) has a unique positive solution σ_B. Indeed, function

$$F(x) = \left\langle \frac{\sigma-x}{\sigma+(d-1)\,x} \right\rangle \tag{46}$$

is obviously decreasing. Also $F(0)=1$ and $F(x)\to -\frac{1}{d-1}$ as $x\to\infty$ which implies the existence and the uniqueness of the solution. We next find the expansion of σ_B in terms of the moments of the disorder parameter $u=\frac{\sigma-\langle\sigma\rangle}{\langle\sigma\rangle}$. It is convenient to introduce new dimensionless variables

$$\eta = \frac{\sigma}{\langle\sigma\rangle}, \qquad \xi = \frac{\sigma_B}{\langle\sigma\rangle}. \tag{47}$$

Obviously $u=\eta-1$. In the new variables Bruggeman's equation (45) takes the form

$$\left\langle \frac{\eta-\xi}{\eta+\delta\xi} \right\rangle = 0, \tag{48}$$

where $\delta = d-1$. Notice that

$$\begin{aligned} \frac{\eta-\xi}{\eta+\delta\xi} &= \frac{1-\xi}{1+\delta\xi} + \frac{(\delta+1)\,\xi(\eta-1)}{(1+\delta\xi)(\eta+\delta\xi)} \\ &= \frac{1-\xi}{1+\delta\xi} + \frac{d\xi\, u}{(1+\delta\xi)^2}\cdot \sum_{n=0}^{\infty} (-1)^n \left(\frac{u}{1+\delta\xi}\right)^n. \end{aligned} \tag{49}$$

After the averaging of the both sides in (49) we get

$$\left\langle \frac{\eta-\xi}{\eta+\delta\xi} \right\rangle = \frac{1-\xi}{1+\delta\xi} + \frac{d\xi}{1+\delta\xi}\cdot \sum_{n=0}^{\infty} (-1)^n \frac{\langle u^{n+1}\rangle}{(1+\delta\xi)^{n+1}} = 0 \tag{50}$$

which together with $\langle u\rangle=0$ immediately implies

$$\frac{1}{\xi}=1+d\sum_{n=2}^{\infty}(-1)^n\frac{\langle u^n\rangle}{(1+\delta\xi)^n}. \tag{51}$$

If the random variable u is small enough the solution of equation (51) can be written as a convergent expansion in terms of the moments of u:

$$\xi=1+\sum_{k=2}^{\infty}\sum_{m=1}^{[\frac{k}{2}]}\sum_{\substack{s_1,\dots,s_m\geqslant 2\\ s_1+\cdots+s_m=k}} b^d_{s_1,\dots,s_m}\langle u^{s_1}\rangle\cdots\langle u^{s_m}\rangle. \tag{52}$$

Notice that this expansion has similar structure to the expansion (6). Easy calculation leads to the following expansion up to the terms of 6th order:

$$\begin{aligned}\xi^{(6)}&=1-\frac{1}{d}\langle u^2\rangle+\frac{1}{d^2}\langle u^3\rangle-\frac{1}{d^3}\langle u^4\rangle-\frac{d-2}{d^3}\langle u^2\rangle^2+\frac{1}{d^4}\langle u^5\rangle\\ &\quad+\frac{3d-5}{d^4}\langle u^2\rangle\langle u^3\rangle-\frac{1}{d^5}\langle u^6\rangle-\frac{4d-6}{d^5}\langle u^2\rangle\langle u^4\rangle\\ &\quad-\frac{2d-3}{d^5}\langle u^3\rangle^2-\frac{2d^2-8d+7}{d^5}\langle u^2\rangle^3,\end{aligned} \tag{53}$$

which gives the 6th order approximation for the Bruggeman approximation

$$\sigma_B^{(6)}=\langle\sigma\rangle\,\xi^{(6)} \tag{54}$$

and its 2D version

$$\begin{aligned}\sigma_B^{(6)}&=\langle\sigma\rangle(1-\tfrac{1}{2}\langle u^2\rangle+\tfrac{1}{4}\langle u^3\rangle-\tfrac{1}{8}\langle u^4\rangle+\tfrac{1}{16}\langle u^5\rangle+\tfrac{1}{16}\langle u^2\rangle\langle u^3\rangle\\ &\quad-\tfrac{1}{32}\langle u^6\rangle-\tfrac{1}{16}\langle u^2\rangle\langle u^4\rangle-\tfrac{1}{32}\langle u^3\rangle^2+\tfrac{1}{32}\langle u^2\rangle^3).\end{aligned} \tag{55}$$

3.3. Effective Conductivity and the Bruggeman Approximation

It follows from (33), (53), (54) that the Bruggeman approximation σ_B coincides with the effective conductivity σ_e up to the terms of 3rd order. However if $d\geqslant 3$ the 4th order terms are different. Let us assume that

$$|u|\leqslant\epsilon,\qquad \langle u^2\rangle\geqslant c\epsilon^2. \tag{56}$$

Then,

$$\sigma_e - \sigma_B = \langle\sigma\rangle\left(\frac{1-H(d)}{d^3}\langle u^2\rangle^2 + O(\epsilon^5)\right)$$

$$\geqslant \langle\sigma\rangle\left(\frac{1-H(d)}{d^3}c^2\epsilon^4 + O(\epsilon^5)\right). \tag{57}$$

This implies that for ϵ small enough $\sigma_e > \sigma_B$. In the 2D case the Bruggeman approximation is even more accurate. It coincides with σ_e up to the 4th order terms. Nevertheless, if $\langle\sigma^3\rangle$ does not vanish then σ_e differs from σ_B in the 5th order. Assume that (56) holds and in addition $|\langle u^3\rangle| \geqslant c\epsilon^3$. Then,

$$\sigma_e - \sigma_B = \langle\sigma\rangle((I - \tfrac{1}{16})\langle u^2\rangle\langle u^3\rangle + O(\epsilon^6)). \tag{58}$$

Since $I > \frac{1}{16}$ we have $\sigma_e \neq \sigma_B$ for ϵ small enough. Notice that σ_B is bigger than σ_e if $\langle u^3\rangle$ is negative. Finally we consider the symmetric 2D case. We shall assume that u satisfies (56) and $\langle u^3\rangle = 0$. Then,

$$\sigma_e - \sigma_B = \langle\sigma\rangle(\tfrac{3}{2}(\tfrac{1}{16} - I)\langle u^2\rangle\langle(u^2 - \langle u^2\rangle)^2\rangle + O(\epsilon^7)). \tag{59}$$

It follows from (59) that $\sigma_e < \sigma_B$ if $\langle(u^2 - \langle u^2\rangle)^2\rangle$ is of the order of ϵ^4 and ϵ is small enough. We summarise all three cases in the following simple proposition.

Proposition 2.

1. Consider the case $d \geqslant 3$. If u satisfies (56) then there exists $\epsilon(d, c) > 0$ such that $\sigma_e > \sigma_B$ for all $\epsilon \leqslant \epsilon(d, c)$.

2. Let $d = 2$, u satisfies (56) and $|\langle u^3\rangle| \geqslant c\epsilon^3$. Then there exists $\epsilon(c) > 0$ such that $\sigma_e \neq \sigma_B$ for all $\epsilon \leqslant \epsilon(d, c)$ and $\operatorname{sgn}(\sigma_e - \sigma_B) = \operatorname{sgn}(\langle u^3\rangle)$.

3. Let $d = 2$ and $\langle u^3\rangle = 0$. If u satisfies (56) and $\langle(u^2 - \langle u^2\rangle)^2\rangle \geqslant c\epsilon^4$ then there exists $\bar{\epsilon}(c) > 0$ such that $\sigma_e < \sigma_B$ for all $\epsilon \leqslant \bar{\epsilon}(c)$.

The following corollary follows easily from Proposition 2. Consider the n-component system where σ takes the values $\sigma_1, \sigma_2,..., \sigma_n$ with probabilities $p_1, p_2,..., p_n$, $p_i > 0$, $p_1 + p_2 + \cdots + p_n = 1$. We shall also assume that the system is irreducible, i.e., $\sigma_i \neq \sigma_j$, $1 \leqslant i, j \leqslant n$. Denote $p_{\min} = \min(p_1, p_2,..., p_n)$.

Corollary 1.

1. Let $d \geqslant 3$. If $|u| \leqslant \epsilon(d, p_{\min})$ then $\sigma_e > \sigma_B$.

2. Let $d=2$. Assume that $n=2$ and $p_1>p_2$. Then $\sigma_e\neq\sigma_B$ provided $|u|\leqslant\epsilon(c)$, where $c=p_2(1-(\frac{p_2}{p_1})^2)$. Moreover, if $\sigma_2>\sigma_1$ then $\sigma_e>\sigma_B$. In the opposite case, i.e., when $\sigma_1>\sigma_2$ one has $\sigma_B>\sigma_e$.

3. Let $d=2$. Assume that $n=3$ and $\langle u^3\rangle=0$. Then there exists $c_1(p_1,p_2,p_3)>0$ such that $\sigma_e<\sigma_B$ if $|u|\leqslant\bar{\epsilon}(c_1)$. In particular, if $\sigma_1=1+\epsilon$, $\sigma_2=1$, $\sigma_3=1-\epsilon$ and $p_1=p_3=p$, $p_2=1-2p$, $0<p<\frac{1}{2}$ then $c_1(p_1,p_2,p_3)=2p(1-2p)$ and $\sigma_e<\sigma_B$ under condition $|u|\leqslant\bar{\epsilon}(2p(1-2p))$.

Finally, we conjecture that for n-component systems the effective conductivity coincides with the Bruggeman approximation only if the probability distribution $\{\sigma\}$ is almost self-dual, see (36).

4. CONCLUDING REMARKS

1. We have derived the exact formulae for the first 5 orders of the expansion of the effective conductivity in terms of the moments of the disorder parameter u in arbitrary dimension. In the 2D case we have also found the 6th order terms. It is quite interesting to extend these results to other types of 2D lattices and to the continuous plaquetes systems. Notice that our duality analysis holds for the general 2D case. Hence, if the expansion (6) is valid, it is enough to find a_3^2, a_5^2, $a_{2,3}^2$ in order to determine all other terms up to the 6th order.

2. We have shown that Bruggeman's solution (55) gives a remarkably accurate approximation for the effective conductivity of the 2D random many-component lattice wire system. It turns out that in the case of square lattice the first four orders of the expansion of Bruggeman's solution in terms of the moments of the disorder parameter coincide with the corresponding expansion of the exact solution. However, in the 5th order the Bruggeman approximation deviates from the exact one. An interesting and natural problem is to verify whether such behaviour is characteristic for the square lattice or it also holds for other 2D lattices. It is also interesting to analyse the relation between Bruggeman's solution and effective conductivity for the continuous 2D random composites. Recently four isotropic three-component S_3-permutation invariant regular structures with three-fold rotation lattice symmetries in the 2D case were treated numerically.[14] A simple cubic equation with one free parameter $A\geqslant 0$

$$\sigma_e^3+AJ_1\sigma_e^2-AJ_2\sigma_e-J_3=0,\qquad J_1=\sum_{i=1}^{3}\sigma_i,\qquad J_2=\sum_{i\neq j}\sigma_i\sigma_j,\qquad J_3=\sigma_1\sigma_2\sigma_3$$

was proposed as an algebraic equation of minimal order. Its solution share many properties with σ_e and corresponds to Bruggeman's solution when

$A = \frac{1}{3}$. The numerically estimated values of A corresponding to different cases were calculated with a very high precision. It appears that they are distinct and lie rather far from $\frac{1}{3}$ for some of the structures. This indicates a strong dependence of σ_e on plane symmetries in contrast with the two-component case.

3. Recently in the paper by Kamenshchik and Khalatnikov[15] the perturbation theory was developed for the periodic three-component plaquetes lattice systems with two-fold rotation lattice symmetry. We hope that their technique combined with our approach will lead to the exact expansion for the effective conductivity in the random plaquetes situation.

4. After the paper was submitted we were informed about the paper by Luck[16] where very similar results were obtained using different method for calculating an expansion for the effective conductivity. In our opinion the approach we use has certain advantages. First of all, it is rigorous and, hence, more suitable for mathematical audience. Secondly, it gives arbitrary good rigorous bounds for the effective conductivity (see (7)).

5. ACKNOWLEDGMENTS

The authors would like to thank A. Kamenshchik and I. Khalatnikov for useful discussions. We are also grateful to Jean-Marc Luck for bringing his paper (ref. 16) to our attention and to D. Khmelev for his help with numerical calculations. The main part of the paper has been written during the stay of one of the authors (LGF) at the Isaac Newton Institute for Mathematical Sciences and its hospitality is highly appreciated. The work was supported in part by grants from the Tel Aviv University Research Authority and the Gileadi Fellowship program.

REFERENCES

1. S. M. Kozlov, The averaging of random operators, *Mat. Sb.* **109(151)**:188 (1979).
2. G. Papanicolaou and S. R. S. Varadhan, Boundary value problems with rapidly oscillating coefficients, in *Colloquia mathematica societatis Janos Bolyai*, Vol. 27, Random fields, v.2 (North-Holland, 1981).
3. V. V. Zhikov, S. M. Kozlov, and O. A. Oleinik, *G*-convergence of parabolic operators, *Russian Math. Surveys* **36**:11 (1981).
4. V. V. Anshelevich, K. M. Khanin, and Ya. G. Sinai, Symmetric random walks in random environments, *Comm. Math. Phys.* **85**:449 (1982).
5. D. J. Bergman, The dielectric constant of a composite material—a problem in classical physics, *Phys. Rep. C* **43**:377 (1978).
6. G. W. Milton, Bounds on the transport and optical properties of a two-component composite material, *J. Appl. Phys.* **52**:5294 (1981).
7. K. Golden and G. Papanicolaou, Bounds for effective parameters of heterogeneous media by analytic continuation, *Comm. Math. Phys.* **90**:473 (1983).

8. O. Bruno and K. Golden, Interchangeability and bounds for the effective conductivity of the square lattice, *J. Stat. Phys.* **61**:361 (1990).
9. A. R. Day and M. F. Thorpe, The spectral function of random resistor networks, *J. Phys.* **8**:4389 (1996).
10. J. B. Keller, A theorem of the conductivity of a composite medium, *J. Math. Phys.* **5**:548 (1964).
11. A. M. Dykhne, Conductivity of a two-dimensional two-phase system, *Sov. Phys. JETP* **32**:63 (1970).
12. P. Kogut and J. Straley, The bicritical macroscopic conductivity exponent in dimensionalities two, three and infinity, *J. Phys. C* **12**:1 (1979).
13. D. A. G. Bruggeman, Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen, *Ann. Phys. (Leipzig)* **24**:636 (1935).
14. L. G. Fel, V. Sh. Machavariani, and D. J. Bergman, Isotropic conductivity of two-dimensional three-component symmetric composites, *J. Phys. A* **33**:6669 (2000).
15. I. M. Khalatnikov and A. Kamenshchik, A diagram technique for perturbation theory calculations of the effective conductivity of two-dimensional systems, *JETP* **91**:1261 (2000).
16. J. M. Luck, Conductivity of random resistor networks: An investigation of the accuracy of the effective-medium approximation, *Phys. Rev. B* **43**:3933 (1991).