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THE CALCULATION OF THE EFFECTIVE VALUES OF PHYSICAL PROPERTIES FOR RANDOM COMPOSITES WITH CIRCULAR INCLUSIONS

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Abstract—The aim of this work is to calculate the effective values of linear physical properties, which are described by tensors of the second rank, for composite materials. Properly chosen mathematical tools of statistics, such as correlation and probability density functions, geometrical information as well as optimum upper and lower bounds, are applied to calculate the effective values of the physical tensor properties, such as the electrical and thermal conductivity, in random systems consisting of two or more phases. Such systems are called composites.

Keywords: Random composite, circular inclusion, Poisson model, correlation function, optimum bounds.

1. INTRODUCTION

In this work the basic statistical ensemble, the tensor properties of which are computed, is physically represented by a composite consisting of two phases, the first one called the matrix phase and the second one the phase of the inclusions. The inclusions are distributed randomly in the matrix and they may form configurations of two or more intersecting areas. For the same purpose the correlation functions are being calculated within the framework of the Poisson model taking account of the geometrical shape of the inclusions (see Sections 2 and 3). Ultimately, use is made of optimum upper and lower bounds for statistically homogeneous and isotropic media (see Sections 4 and 5).

One relates the correlation functions to some probability density function, here the Poisson function, governing the configurations of two or more inclusions. The method of computing correlation functions taking into account the geometrical shape of the inclusions as well as material factors, is a new branch of science based on original works of Matheron [5], Serra [6, 7] and others, called mathematical morphology.

In the present paper explicit calculations of the one-, two- and three-point correlation functions are performed considering the inclusions to be circular areas for the two-dimensional case. The inclusions correlate to each other with the common geometrical area of intersection. Thus the center-to-center distance defines a correlation length the variation of which estimates the extent of the correlation effects. The geometrical configurations of two or three intersecting circular inclusions are described analytically and exact results are presented.

As referred to here, the property of electrical or heat conductivity, which we denote with the greek symbol $\hat{\sigma}$, is considered to be a function of cartesian coordinates $\mathbf{r}$, namely $\hat{\sigma}(\mathbf{r})$. Such functions, which we call structure functions, can be defined for all tensor properties. The tensor field of the electrical (or heat) conductivity describes the distribution of the property over the matrix phase as well as over the various inclusions of the composite.

It will be assumed further that the composite is statistically homogeneous and isotropic, that is

$$\langle\hat{\sigma}(\mathbf{r}_1)\ldots\hat{\sigma}(\mathbf{r}_n)\rangle = \langle\hat{\sigma}(\mathbf{r}_1+\mathbf{r})\ldots\hat{\sigma}(\mathbf{r}_n+\mathbf{r})\rangle$$

and

$$\langle\hat{\sigma}(\mathbf{r}_1)\ldots\hat{\sigma}(\mathbf{r}_n)\rangle = \langle[D_{\vartheta,\varphi,\psi}\hat{\sigma}(\mathbf{r}_1)]\ldots[D_{\vartheta,\varphi,\psi}\sigma(\mathbf{r}_n)]\rangle.$$

($D_{\vartheta,\varphi,\psi}$ is a torsional operator, ϑ, φ, ψ are the Euler angles).

The effective value of the property denoted by $\hat{\sigma}^{\text{eff}}$ is determined within optimum upper and lower bounds obtained from a series, which includes terms with correlation functions of all orders up to infinity. The series has the form

$$\hat{\sigma}^{\text{eff}} = \langle\hat{\sigma}\rangle - \langle\hat{\sigma}'\vec{\Gamma}\hat{\sigma}'\rangle + \langle\hat{\sigma}'\vec{\Gamma}\hat{\sigma}'\vec{\Gamma}\hat{\sigma}'\rangle - \cdots + \cdots$$

For further details about this series the reader should consult Ref. 1. $\vec{\Gamma}$ is the modified Green function, also a tensor of the 2nd rank, obtained from the Green function as:

$$\Gamma_{ij}(\mathbf{r}_1,\mathbf{r}_2) = \partial_i\partial_j G(\mathbf{r}_1,\mathbf{r}_2);$$

$\hat{\sigma}'$ is the deviation from the mean: $\hat{\sigma}' = \hat{\sigma} - \langle\hat{\sigma}\rangle$. Here $G(\mathbf{r}_1,\mathbf{r}_2) = 1/(4\pi\sigma_0|\mathbf{r}_1-\mathbf{r}_2|)$, which is the solution of the Poisson equation.

With double differentiation one obtains for the modified Green function in three-dimensional space:

$$\Gamma_{ij}(\mathbf{r}_1,\mathbf{r}_2) = E_{ij}\delta(\mathbf{r}_1,\mathbf{r}_2) - F_{ij}(\vartheta,\varphi)/|\mathbf{r}_1-\mathbf{r}_2|^3.$$

The angles ϑ, φ are related to the vectorspace about $|\mathbf{r}_1 - \mathbf{r}_2|$. $E_{ij} = \delta_{ij}/(3\sigma_0)$ is the local and $F_{ij} = (\delta_{ij} - 3e_i e_j)/(4\pi\sigma_0)$, expressed in cartesian coordinates, the non-local part of Γ. $\mathbf{e}_i$, $\mathbf{e}_j$ are the unit vectors and δ_{ij} the Kronecker symbol. The ensemble averages with the notation $\langle\ \rangle$ as well as the effective value $\tilde{\sigma}^{\text{eff}}$ do not depend on position in the macrohomogeneous case. σ_0 is the material constant of an isotropic and homogeneous reference medium, equal to the average value of $\tilde{\sigma}$, that is $\sigma_0 = \langle\sigma\rangle$.

There exist two general bound theorems in this series; one, due to Dederichs and Zeller [8], yields the bounds of odd order; the other, due to Kröner [1], those of even order. Such bounds exploit statistical information given in terms of correlation functions up to order n and will be denoted by $\sigma^{(\pm n)}$. The sign "+" indicates that it is an upper and "−" a lower bound for $n = 1, 2, 3, \ldots$. Normally one is content with bounds of low order, i.e. $n \leqslant 3$. The bound $\sigma^{(+1)}$ is that of Voigt [9] and $\sigma^{(-1)}$ that of Reuss [10]. The bounds $\sigma^{(+2)}$ and $\sigma^{(-2)}$ are those of Hashin and Strikman [11]. The bounds $\sigma^{(+3)}$ and $\sigma^{(-3)}$ given by Kröner in [13] have a complicated form (see [12, 13]). A detailed presentation of the theoretical point of view as well as numerical calculations of bounds of third order for circular inclusions compose this article. The results obtained here represent an extension to those of Voigt–Reuss and Hashin–Strikman with which they are finally compared in a graph.

2. THE CORRELATION FUNCTIONS

For a two-phase statistically homogeneous and isotropic structure with isotropic and homogeneous phases one defines the following mathematical elements:

(a) Two (constant) material parameters σ_1 and σ_2, the first one defined in phase 1 and the second one in phase 2. The distribution of the physical property of electrical or heat conductivity is homogeneous over the two phases.

(b) Two so-called indicatrices are defined as

$$k_1(\mathbf{r}) = \begin{cases} 1 & \text{at } \mathbf{r} \text{ in the phase 1} \\ 0 & \text{elsewhere} \end{cases}$$

$$k_2(\mathbf{r}) = \begin{cases} 1 & \text{at } \mathbf{r} \text{ in the phase 2} \\ 0 & \text{elsewhere} \end{cases} \tag{1}$$

Over the entire phasefield the relation

$$k_1(\mathbf{r}) + k_2(\mathbf{r}) = 1 \tag{2}$$

is valid, and more generally

$$\sum_i k_i(\mathbf{r}) = 1.$$

Therefore it is sufficient to prescribe one indicatrix for a two-phase material. Moreover,

$$\int k_1(\mathbf{r})\mathrm{d}A_1 = A_1,$$

$$\int k_2(\mathbf{r})\mathrm{d}A_2 = A_2, \quad (A_1 + A_2 = A) \tag{3}$$

with A_1 and A_2 the areas of the two phases. One can easily see that both functions $k_1(\mathbf{r})$ and $k_2(\mathbf{r})$ relate to the area fractions of the composite. Regarding one ensemble of materials one gets:

$$\langle k_1(\mathbf{r})\rangle = A_1/A, \quad \langle k_2(\mathbf{r})\rangle = A_2/A, \tag{4}$$

using the symbol $\langle \ldots \rangle$ to indicate averaging over the ensemble, so far as the distribution of the material parameters are statistically homogeneous. If both relations (3) and (4) are simultaneously valid, one obtains an expression for the ergodic hypothesis. This basic principle of statistical physics, which will be repeatedly used in this work, states briefly that the ensemble averages are equal to the area (volume) averages.

(c) The two-point correlation function $\langle\sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h})\rangle$, with $\mathbf{h}$ as a displacement in space, or more specifically, if we consider circular inclusions, means the center-to-center vector of two correlated inclusions.

The material function $\sigma(\mathbf{r})$ will be expressed by the indicatrices $k_1(\mathbf{r})$ and $k_2(\mathbf{r})$. Using (3) one gets:

$$\langle\sigma(\mathbf{r})\rangle = \sigma_1\langle k_1(\mathbf{r})\rangle + \sigma_2\langle k_2(\mathbf{r})\rangle$$

$$\langle\sigma(\mathbf{r}+\mathbf{h})\rangle = \sigma_1\langle k_1(\mathbf{r}+\mathbf{h})\rangle + \sigma_2\langle k_2(\mathbf{r}+\mathbf{h})\rangle. \tag{5}$$

One generally obtains for the correlation function of second order:

$$\langle\sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h})\rangle = \sum \sigma_i\sigma_j C_{ij}(\mathbf{h}) \quad (i,j = 1, 2) \tag{6}$$

which is valid for more than two phases. $C_{ij}(\mathbf{h})$ is called the covariance function. It is given as:

$$C_{ij}(\mathbf{h}) = \langle k_i(\mathbf{r})k_j(\mathbf{r}+\mathbf{h})\rangle. \tag{7}$$

For the calculation of the two-point correlation functions the covariances C_{11}, C_{22}, C_{12} are needed. C_{11} and C_{12} are expressed by C_{22}, and with eqns (4) and (7) the following relations are obtained:

$$C_{22}(\mathbf{h}) = \langle k_2(\mathbf{r})k_2(\mathbf{r}+\mathbf{h})\rangle \tag{8}$$

$$C_{11}(\mathbf{h}) = \langle k_1(\mathbf{r})k_1(\mathbf{r}+\mathbf{h})\rangle = 1 - 2\frac{A_2}{A} + C_{22}(\mathbf{h}) \tag{9}$$

$$C_{12}(\mathbf{h}) = \langle k_1(\mathbf{r})k_2(\mathbf{r}+\mathbf{h})\rangle = \frac{A_2}{A} - C_{22}(\mathbf{h}). \tag{10}$$

At this point a brief reference to the Poisson model is made according to which the probability density function can be defined (for further information see [2, 3]). One thinks of two-dimensional space, in which points are defined. These points are distributed randomly and uncorrelated. Theoretically one attributes a physical quantity to each point. For reasons of practicality it is less cumbersome if one makes use of an infinitesimal area of points dr^2 and simultaneously defines a density ρ, which is a constant independent of $\mathbf{r}$. In the Poisson model, presuming homogeneity in space, the points are supposed to be centers of the so-called Poisson cells, which grow symmetrically in time and space, so that they can be considered as circular inclusions, in the ideal case. They can also intersect among themselves. Under this assumption one writes a Poisson probability density function for the case that configurations of two intersecting inclusions appear:

$$C_{22}(\mathbf{h}) = \exp\{-\rho A(\mathbf{h})\}. \tag{11}$$

ρ is the Poisson point-density and A is the common area of the intersecting circular inclusions (see also [4], p. 82). Substituting eqn (11) in eqns (9), (10) and also in (6) one has:

$$\langle \sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h})\rangle = \alpha + \beta \exp\{-\rho A(\mathbf{h})\}, \tag{12}$$

where

$$\alpha = \sigma_1^2 - 2\sigma_1(\sigma_1 - \sigma_2)\frac{A_2}{A},$$

$$\beta = (\sigma_1 - \sigma_2)^2.$$

The model also applies to spherical inclusions, if one makes slight changes in the above formulae, substituting volumes for areas. What is needed, however, is the deviation formulae rather than only the correlation functions. The deviation of second order is written as:

$$\langle \sigma'(\mathbf{r})\sigma'(\mathbf{r}+\mathbf{h})\rangle = \langle \sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h})\rangle - \langle\sigma\rangle^2. \tag{13}$$

In analogy to the two-point correlation functions the three-point correlation functions are constructed for the case that three inclusions correlate to each other:

$$\langle \sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h}_1)\sigma(\mathbf{r}+\mathbf{h}_2)\rangle = \sum \sigma_i\sigma_j\sigma_k C_{ijk}(\mathbf{h}_1, \mathbf{h}_2) \quad (i,j,k = 1,2). \tag{14}$$

Or more explicitly:

$$\langle \sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h}_1)\sigma(\mathbf{r}+\mathbf{h}_2)\rangle = \sigma_1^3 C_{111}(\mathbf{h}_1, \mathbf{h}_2) + 3\sigma_1^2\sigma_2 C_{121}(\mathbf{h}_1, \mathbf{h}_2) + 3\sigma_1\sigma_2^2 C_{212}(\mathbf{h}_1, \mathbf{h}_2) + \sigma_2^3 C_{222}(\mathbf{h}_1, \mathbf{h}_2). \tag{15}$$

The covariance functions for three points C_{111}, C_{121}, C_{212} are expressed by C_{222}, and one obtains for the three-point correlation function:

$$\langle \sigma(\mathbf{r})\sigma(\mathbf{r}+\mathbf{h}_1)\sigma(\mathbf{r}+\mathbf{h}_2)\rangle = \gamma + \delta C_{22}(\mathbf{h}_1) + \sigma_1 C_{22}(\mathbf{h}_2) + \epsilon C_{22}(\mathbf{h}_3) - \zeta C_{222}(\mathbf{h}_1, \mathbf{h}_2), \tag{16}$$

where $\mathbf{h}_1$, $\mathbf{h}_2$ are the center-to-center vectors of three correlated circular inclusions. Further

$$\gamma = \sigma_1^3 - 3\sigma_1^2(\sigma_1 - \sigma_2)\frac{A_2}{A}$$

$$\delta = \sigma_1^3 - 3\sigma_1^2\sigma_2 + 3\sigma_1\sigma_2^2$$

$$\epsilon = \sigma_1^2(\sigma_1 - 3\sigma_2)$$

$$\zeta = (\sigma_1 - \sigma_2)^3.$$

The deviation of third order is then $\langle \sigma'(\mathbf{r})\sigma'(\mathbf{r}+\mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_2)\rangle$:

$$\langle \sigma'(\mathbf{r})\sigma'(\mathbf{r}+\mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_2)\rangle = [\gamma - 3\alpha\langle\sigma\rangle + 2\langle\sigma\rangle^3 + (\delta + \beta\langle\sigma\rangle)C_{22}(\mathbf{h}_1) + (\sigma_1^3 - \beta\langle\sigma\rangle)C_{22}(\mathbf{h}_2) + (\epsilon - \beta\langle\sigma\rangle)C_{22}(\mathbf{h}_3) - \zeta C_{222}(\mathbf{h}_1, \mathbf{h}_2)]. \tag{17}$$

Under the same assumption as for [11] a Poisson probability density function for the case that three circular inclusions may intersect is written as:

$$C_{222}(\mathbf{h}_1, \mathbf{h}_2) = \exp\{-\rho A(\mathbf{h}_1, \mathbf{h}_2)\}. \tag{18}$$

3. THE GEOMETRICAL CONFIGURATIONS OF THE CIRCULAR INCLUSIONS

Let us first consider the case when two circular inclusions correlate to each other. They may intersect or touch each other. Let the correlation length be the center-to-center vector $\mathbf{h}$, with $|\mathbf{h}| \leqslant D$, the diameter of the circles which we consider to be equal for all inclusions. For the case of two intersecting circular inclusions their geometrical common area on the plane is needed, as shown in Fig. 1.

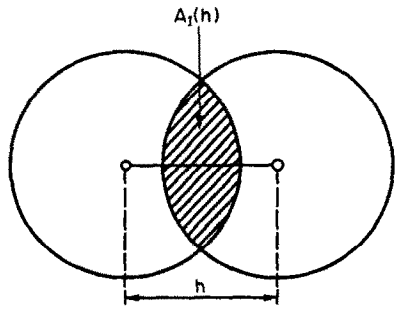

Fig. 1. Intersection of two circular areas.

This area is given by the function:

$$A_c(\mathbf{h}) = 2A(0) - A_I(\mathbf{h}); \tag{19}$$

$A_c(\mathbf{h})$ is the geometrical common area of two circles, $A(0)$ is the area when the centers of the two circles coincide and this happens if $|\mathbf{h}| = 0$ and $A_I(\mathbf{h})$ is the area of intersection.

For the case when three circular inclusions intersect, three correlation lengths $|\mathbf{h}_1|$, $|\mathbf{h}_2|$, $|\mathbf{h}_3| \leqslant D$ are defined, which are the sides of a triangle, whose three points are the centers of the circles. The common area is then:

$$A_c(\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3) = 3A(0) - A_I(\mathbf{h}_1) - A_I(\mathbf{h}_2) - A_I(\mathbf{h}_3) + A_{cI}(\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3). \tag{20}$$

A_c is the common area of the three circular inclusions, $A_I(\mathbf{h}_1)$, $A_I(\mathbf{h}_2)$, $A_I(\mathbf{h}_3)$ are the three areas of intersection and $A_{cI}(\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3)$ is the common area of the three areas of intersection, as shown in Fig. 2.

In order to avoid complications related to the definition of a coordinate system at the center or outside a circle area, all formulae for the calculated areas have been expressed by two parameters, the diameter D which is constant and the correlation length $|\mathbf{h}| \equiv h$, which is a variable.

After formal algebraic computations the area of intersection for two circles is found to be [14]:

$$A_I(h) = \frac{D^2}{2}\arccos\left(\frac{h}{D}\right) - \frac{h}{2}\sqrt{D^2 - h^2}, \quad h \equiv |\mathbf{h}|. \tag{21}$$

The common area according to eqn (19) is given by

$$A_c(h) = A(0) - A_I(h) = \frac{\pi D^2}{2} - \frac{D^2}{2}\arccos\left(\frac{h}{D}\right) + \frac{h}{2}\sqrt{D^2 - h^2}. \tag{22}$$

The case of three intersecting circular inclusions is more complicated. One has three geometrical areas of intersection given by relation (21) depending on $h_1 \equiv |\mathbf{h}_1|$, $h_2 \equiv |\mathbf{h}_2|$, $h_3 \equiv |\mathbf{h}_3|$ as follows:

$$A_I(h_1) = \frac{D^2}{2}\arccos\left(\frac{h_1}{D}\right) - \frac{h_1}{2}\sqrt{D^2 - h_1^2} \tag{23}$$

$$A_I(h_2) = \frac{D^2}{2}\arccos\left(\frac{h_2}{D}\right) - \frac{h_2}{2}\sqrt{D^2 - h_2^2} \tag{24}$$

$$A_I(h_3) = \frac{D^2}{2}\arccos\left(\frac{h_3}{D}\right) - \frac{h_3}{2}\sqrt{D^2 - h_3^2}. \tag{25}$$

The difficulty arises if one tries to calculate the last term A_{cI} in eqn (20). This term cannot be expressed in a simple formula, at least according to the method followed here, because it is derived from the integral form (see also Fig. 2):

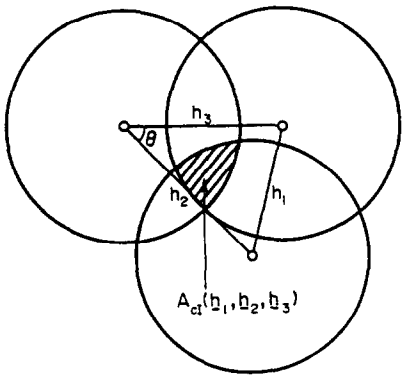

Fig. 2. The general case of three circular intersection areas.

$$A_{cI} = \int_{x_1}^{x_2} y_2(x)\,dx + \int_{x_3}^{x_2} y_1(x)\,dx - \int_{x_3}^{x_1} y_3(x)\,dx \tag{26}$$

with

$$y_1(x) = \pm\sqrt{\frac{D^2}{4} - x^2}$$

$$y_2(x) = \pm\sqrt{\frac{D^2}{4} - (x - x_{02})^2}$$

$$y_3(x) = y_{03} \pm \sqrt{\frac{D^2}{4} - (x - x_{03})^2}.$$

The equations above define three circular inclusions centered at (x_{01}, y_{01}), (x_{02}, y_{02}), (x_{03}, y_{03}). The first circle is centered at $x_{01} = 0$, which is equivalent to assumption of homogeneity. The integration boundaries are determined using analytic geometry and are functions of the plane coordinates expressed in relative coordinates h_1, h_2, h_3 so that they take a very complicated form [14]. This is the reason why the A_{cI} term will be calculated numerically. A computer program was set up, a part of which computes this integral form. The common area of three intersecting circular inclusions is given by:

$$A_c(h_1, h_2, h_3) = \frac{D^2}{2}\left[\frac{3\pi}{2} - \arccos\left(\frac{h_1}{D}\right) - \arccos\left(\frac{h_2}{D}\right) - \arccos\left(\frac{h_3}{D}\right)\right] + \tfrac{1}{2}(h_1\sqrt{D^2 - h_1^2} + h_2\sqrt{D^2 - h_2^2} + h_3\sqrt{D^2 - h_3^2}) + A_{cI}(h_1, h_2, h_3). \tag{27}$$

The calculated common areas are inserted into the Poisson distribution functions (11) and (18) for each case, respectively.

4. THE OPTIMUM UPPER AND LOWER BOUNDS FOR STATISTICALLY HOMOGENEOUS AND ISOTROPIC MEDIA

The effective values σ^{eff} of the electrical or heat conductivity will be calculated using the optimum bound of first and third order showing that σ^{eff} can be determined more exactly within the third order bounds.

The upper and lower bounds of first order are those of Voigt and Reuss given by the mean value of the structure function σ as follows:

$$\sigma^{(+1)} = \langle \sigma \rangle \tag{28}$$

$$\sigma^{(-1)} = \left\langle \frac{1}{\sigma} \right\rangle^{-1} \equiv \langle s \rangle^{-1}, \tag{29}$$

with $s = 1/\sigma$.

Using eqns (4) and (5), the mean value $\langle \sigma \rangle$ is found to be:

$$\langle \sigma \rangle = (\sigma_1 - \sigma_2)\frac{A_1}{A} + \sigma_2. \tag{30}$$

A similar computation gives $\langle s \rangle$ as:

$$\langle s \rangle = \left(\frac{1}{\sigma_1} - \frac{1}{\sigma_2}\right)\frac{A_1}{A} + \frac{1}{\sigma_2}. \tag{31}$$

The third order upper and lower bounds are [13]:

$$\sigma^{(+3)} = \langle \sigma \rangle - \frac{\langle \sigma'(\mathbf{r})\Gamma_{ij}(\mathbf{r}, \mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_1)\rangle}{[\langle \sigma'(\mathbf{r})\Gamma_{ij}(\mathbf{r}, \mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_1)\rangle + \langle \sigma'(\mathbf{r})\Gamma_{ij}(\mathbf{r}, \mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_1)\Gamma_{ij}(\mathbf{r}, \mathbf{h}_2)\sigma'(\mathbf{r}+\mathbf{h}_2)\rangle]} \tag{32}$$

$$\sigma^{(-3)} = \left\{\langle s \rangle - \frac{\langle s'(\mathbf{r})\Delta_{ij}(\mathbf{r}, \mathbf{h}_1)s'(\mathbf{r}+\mathbf{h}_1)\rangle}{[\langle s'(\mathbf{r})\Delta_{ij}(\mathbf{r}, \mathbf{h}_1)s'(\mathbf{r}+\mathbf{h}_1)\rangle + \langle s'(\mathbf{r})\Delta_{ij}(\mathbf{r}, \mathbf{h}_1)s'(\mathbf{r}+\mathbf{h}_1)\Delta_{ij}(\mathbf{r}, \mathbf{h}_2)s'(\mathbf{r}+\mathbf{h}_2)\rangle]}\right\}^{-1}. \tag{33}$$

The modified Green functions $\Gamma_{ij}(r, h_1)$, $\Delta_{ij}(r, h_1)$ are for the two-dimensional case:

$$\Gamma_{ij}(\mathbf{r}, \mathbf{h}_1) = E_{ij}\delta(\mathbf{r}, \mathbf{h}_1) + \frac{F_{ij}(\vartheta)}{h^2} \tag{34}$$

$$\Delta_{ij}(\mathbf{r}, \mathbf{h}_1) = U_{ij}\delta(\mathbf{r}, \mathbf{h}_1) + \frac{V_{ij}(\vartheta)}{h^2}, \tag{35}$$

where

$$E_{ij} = \frac{1}{2\pi\langle \sigma \rangle}\delta_{ij}, \qquad U_{ij} = \frac{1}{2\pi\langle s \rangle}\delta_{ij}.$$

The F_{ij} and V_{ij} terms can be written as functions of spherical coordinates ϑ, φ for the case of spherical inclusions and they reduce to functions of ϑ for the case of circular inclusions. ϑ is the angle of the vectors $\mathbf{h}_2$ and $\mathbf{h}_3$ (Fig. 2).

After having calculated the correlation functions up to order three, and using the ergodic hypothesis the following integral forms are evaluated numerically:

$$\langle \sigma'(\mathbf{r})\Gamma_{ij}(\mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_1)\rangle = \int \Gamma_{ij}(\mathbf{h}_1)\langle \sigma'(\mathbf{r})\sigma'(\mathbf{r}+\mathbf{h}_1)\rangle \, \mathrm{d}h_1^2 \tag{36}$$

$$\langle \sigma'(\mathbf{r})\Gamma_{ij}(\mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_1)\Gamma_{kl}(\mathbf{h}_2)\sigma'(\mathbf{r}+\mathbf{h}_2)\rangle = \int \Gamma_{ij}(\mathbf{h}_1)\Gamma_{kl}(\mathbf{h}_2)\langle \sigma'(\mathbf{r})\sigma'(\mathbf{r}+\mathbf{h}_1)\sigma'(\mathbf{r}+\mathbf{h}_2)\rangle \, \mathrm{d}h_1^2 \, \mathrm{d}h_2^2. \tag{37}$$

Integrals for the inverse problem (33) which determines the lower bounds are evaluated in a similar way.

5. NUMERICAL RESULTS

Integration (36) is simpler than (37), because the symmetrical non-local term results in zero, so that the local term remains as a contribution to (36), which is equal to: $\langle \sigma'(r)\sigma'(r)\rangle E$.

In (37), however, the integral over the non-local term does not vanish and has to be derived numerically. The reason is that the previously obtained Poisson probability density (18) includes the sum of three internal integrals with variable integration upper bounds in the exponent of the function. The only way to calculate these integrals is to construct a computer program which works out the problem numerically. The method used was the recursive Gaussian quadrature with six points in each interval and five intervals for each variable; because the Gaussian quadrature does not take into account the end points of the intervals it is a very suitable method for functions which are in a respect "lightly" singular at the end of the integration interval. Such a case is the function included in (37) [14]:

$$P(\mathbf{h}_1, \mathbf{h}_2, \vartheta) = \frac{\cos\vartheta}{h_1 h_2}\exp\{-\rho A_c(h_1, h_2, \vartheta)\}, \qquad h_1 > 0, \quad h_2 > 0. \tag{38}$$

The integration variables are h_1, h_2, h_3. The variable h_3 can be written according to the cosinus theorem

as: $h_3 = h_1 + h_2 - 2h_1h_2\cos\vartheta$, introducing the angle ϑ between the vectors $\mathbf{h}_1$ and $\mathbf{h}_2$. The bounds for the integration in (37) are

$$\int_0^{nD} \mathrm{d}h_1, \quad \int_0^{mD} \mathrm{d}h_2, \quad \int_0^{\pi} \mathrm{d}\vartheta,$$

with $n \geqslant m$ integer numbers. The integration in (38) reduces to the calculation of

$$P = \int\left[\int\left(\int P(h_1, h_2, \vartheta)\,\mathrm{d}\vartheta\right)\mathrm{d}h_2\right]\mathrm{d}h_1.$$

For explicit results the following assumptions are made: the density $\rho = n/A$ is arbitrarily set equal to one for the case of very low inclusion concentration in the matrix. A more complete computation of the bounds at middle and high concentrations of the inclusions should be desirable. This, however, is a matter for future research. It is assumed further that the diameter D of the circles is equal to one. This value is taken arbitrarily because all formulae, if modified properly, are independent of the diameter D. This fact can become clear by the following discussion. Relation (27) is so modified that all terms depend only on the fractions h_1/D, h_2/D; because h_1, h_2 vary with D as seen in the bounds of the integration ($0 < h_1 < nD$, $0 < h_2 < mD$) the fractions always remain independent of D. The total area A is connected to the inclusions—area A_1, which is a function of D^2 (circular inclusions), by the relation $A = A_1 + A_2$ (A_2 is the matrix area) which means that A is also a function of D^2. This makes (27) independent of D as a whole. For all values of D one always derives the same value of P. This is a remarkable result of the method here.

Performing the integration, the value for P was found to be equal to 1598. In this way the ensemble average (37) has been found to be equal to $\langle\sigma'(\mathbf{r})\sigma'(\mathbf{r})\sigma'(\mathbf{r})\rangle E^2 + P$ and will be set into the denominator of the bounds (32) and (33). The upper and lower bounds of first as well as of second and third order are plotted in Fig. 3, with σ_1 and σ_2 taking the values 0.02 and 1, respectively. These values are arbitrary and it has been found [14] that the smaller their difference the narrower the bounds. The bounds are plotted for the case that homogeneity holds so that they finally depend on the area fraction A_1/A. The area fraction becomes equal to one (the maximal value) if the composite matrix is totally covered with inclusions, so that practically only one phase appears. One can see that the bounds of third order are narrower than the simple first order bounds of Voigt and Reuss. This occurs because the higher the order of the correlation functions taken into account the narrower are the bounds and of course the more exact the outcome.

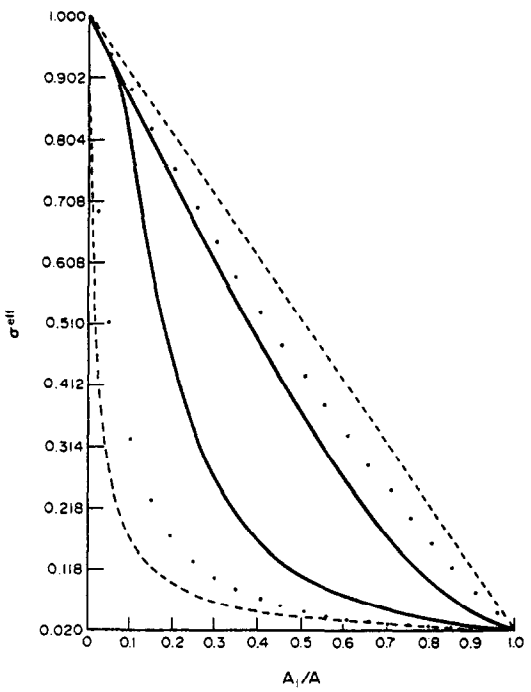

Fig. 3. The optimal bounds of first (– – –), second (· · ·) and third (——) order.

6. CONCLUSION

In this work a method for calculating the effective values of physical properties described by tensors of the 2nd rank has been presented and applied to electrical and heat conductivity. Correlation functions of first, second and third order as well as their deviations have been derived for circular inclusions in a two phase composite. All the expressions obtained through a geometrical calculation of areas give results for the effective values independent of the diameter of the circular inclusions and this represents a major accomplishment.

The effective value σ^{eff} has been computed within the optimum upper and lower bounds of first and third order, under consideration of homogeneity and isotropy for the composite. The bounds become more exact if higher order correlation functions and their deviations are considered. Calculations for higher order terms than the third have not yet been implemented.

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