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Continued fraction representation for the effective thermal conductivity coefficient of a regular two-component composite

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Abstract—A method is given which allows the presentation of the effective conductivity coefficient of a composite with a periodic structure in an analytical form as a continuous fraction expansion. Owing to rapid convergence, only a few levels of the fraction are needed to describe the effective conductivity coefficient with good accuracy. The obtained formula is valid for a wide range of parameters, excluding the asymptotic case when inclusions are very close to touching and the ratio of conductivities of both components tends to infinity. The detailed calculations have been carried out in the two-dimensional case for the square arrays of cylinders.

1. INTRODUCTION

THIS PAPER aims to predict the effective conductivity, λ_{ef}, of a two-phase material which consists of a dispersed phase in the form of a regular array of cylinders embedded in a homogeneous continuous phase referred to as a matrix. Conductivities of the dispersed and continuous phases are given, and are equal to λ_d and λ_c, respectively. The effective conductivity of a composite material is determined by the two non-dimensional parameters: $h = \lambda_d/\lambda_c$ and $\varphi = V_d/V$, where V_d is the volume of the dispersed phase and V is the total volume of the both phases. Although the problem is considered here in the context of thermal conductivity, the results may be applied to other transport properties such as the electric conductivity, dielectric constant, and magnetic permeability, since they all may be considered with the aid of the same mathematical formalism. A more detailed review of the effective transport properties in various fields of physics may be found in the survey articles of Batchelor [1] or Torquato [2].

The effective transport properties of two-phase media has been the subject of investigation for more than 100 years. The first-order approximation in the volume fraction, φ, for the effective conductivity coefficient was obtained by Maxwell [3], who considered each particle of the composite as an isolated dipole. The second-order approximation was due to Rayleigh [4], who took into account particle moments up to the octupole and calculated the effective transport coefficient from a truncated system of linear algebraic equations. The Rayleigh method was then developed for higher order approximations by other authors, mainly for composites with cubic arrays of spherical inclusions. In the 1970s composite materials with regularly spaced cylindrical inclusions again became the subject of interest owing to their new applications, such as absorbers of solar energy [5]. Based on the Rayleigh method, McPhedran, McKenzie, and others from the University of Sydney [6] have evaluated the effective transport coefficient by means of numerical computations, and presented the results in a tabulated form for discrete values of parameters φ and h. In ref. [6] a new analytic formula for the effective transport coefficient has also been given. Asymptotic behaviour for $h \to \infty$ and $\varphi \to \varphi_{max}$ (φ_{max} being the volume fraction corresponding to the touching cylinders) was considered in ref. [7], and an analytic expression for the effective transport coefficient has been derived. However, the formulae from refs. [6] and [7] are of a rather low order approximation, and there still exists some gap where no accurate results are given. A semi-analytic method was applied by McPhedran and Milton [8]; they represented the effective coefficient in the form of power expansion in α: the parameter related to h and defined in Section 2 by equation (26). To get a better convergence McPhedran and Milton approximated the power series by means of rational functions. The coefficients of these functions have been calculated for some discrete values of φ.

An alternative approach to that of Rayleigh has been proposed by Zuzovsky and Brenner [9] and then developed by Sangani and Acrivos [10]. This approach, which is sometimes called the induced sources method, takes advantage of the periodicity of the potential field, and with the use of the Wigner potential [11] avoids some convergence problems that occur in the Rayleigh approach. In refs. [9–11] this method was applied to systems with cubic arrays of spheres. A two-dimensional case was considered by Cichocki and Felderhof [12]. A survey of various cal-

NOMENCLATURE

a	dimensionless radius of cylinders
A_m	Wigner coefficients, S_m/m
b	radius of cylinders
f	volume fraction related to the maximal value, φ/φ_{max}
G_0	macroscopic gradient of temperature [$K\,m^{-1}$]
h	ratio of heat conductivities of the both components, λ_d/λ_c
$\mathbf{i}, \mathbf{j}$	unit vectors in the Cartesian coordinate system
l	dimension of the unit cell
$\mathbf{n}$	unit normal vector
$\mathbf{q}$	heat flux [$W\,m^{-2}$]
r	dimensionless radius in the cylindrical coordinate system
R	radius in the cylindrical coordinate system
$\mathbf{R}_n$	positions of the centres of grid cells
S_m	Rayleigh sums
T	temperature [K]
V	volume [m^3]
x, y	dimensionless Cartesian coordinates
X, Y	Cartesian coordinates.

Greek symbols

α	dimensionless heat conductivity, $(\lambda_c-\lambda_d)/(\lambda_c+\lambda_d)$
β	auxiliary dimensionless parameter characterising the effective conductivity, $\alpha\varphi(1+\mu)/(1-\mu)$
λ	heat conductivity [$W\,m^{-1}\,K^{-1}$]
μ	dimensionless effective conductivity of the composite, λ_{ef}/λ_c
ρ	density of the heat sources distribution
θ	angle in the cylindrical coordinate system
φ	volume fraction of the discrete component.

Subscripts

c, d	continuous and discrete component, respectively
ef	effective value for the composite
max	maximal value
M, P	macroscopic and periodic components of the temperature field.

Superscripts

c, d	continuous and discrete components (of the temperature field).

culation methods of the effective transport coefficient for a regular array of cylinders is given in ref. [13].

Bergman [14] investigated analytical properties of the effective transport coefficient of a macroscopically uniform composite of any given geometrical structure as a function of h in the complex plane. Bergman has shown that the effective coefficient is represented by a function which is analytic everywhere except in some points on the negative part of the real axis, where it has poles of the first order. Such functions, Stieltjes functions, are well known in the literature. One of the advantages of these functions is that they are well approximated by means of continued fractions [15].

On the basis of these functions we present a method to derive the effective coefficient as a function of two arguments α and φ. The function has the form of a continued fraction. It rapidly converges in a wide range of both arguments: thus only a few levels of the fraction are needed to describe the function with good accuracy. The analytic expression so obtained is more accurate than the previous formulae, and together with the asymptotic formula [7] covers the whole range of h and φ.

2. THE GOVERNING EQUATIONS AND THE BOUNDARY CONDITIONS

Consider here a composite consisting of a square array of identical parallel cylinders embedded in a homogeneous medium. The cylinders of radius b are infinitely long and the system may be treated as two-dimensional (Fig. 1). With respect to the periodic structure of the composite we may limit ourselves to a unit cell, which repeats throughout the system. The distance between the cylinder axes is l. The problem will be considered in the cylindrical (R, θ) coordinate system, taking as its origin the centre of a chosen unit cell. We shall also use the Cartesian coordinate system (X, Y). Positions of the centres of grid cells are given by the vector

$$\mathbf{R}_n = l\cdot(n_1\mathbf{i}+n_2\mathbf{j}), \quad n_1, n_2 = 0, \pm 1, \pm 2, \ldots, \quad (1)$$

where $\mathbf{i}$ and $\mathbf{j}$ are the basic unit vectors in X and Y directions, respectively.

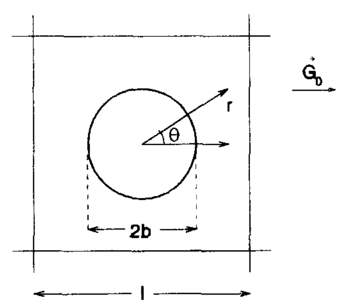

FIG. 1. Elementary cell of a square grid of cylinders.

Throughout this paper the nondimensional coordinates relating to the dimension l of a unit cell will be used:

$$r = R/l, \quad x = X/l, \quad y = Y/l. \tag{2}$$

A steady-state heat conduction can be described by the following equations:

$$\nabla \cdot \mathbf{q}_i = \rho_i \tag{3}$$

$$\mathbf{q}_i = -\lambda_i \cdot \nabla T^i. \tag{4}$$

The first of these equations is a conservation equation for a heat flux $\mathbf{q}_i$, where ρ_i is a given distribution of heat sources. The second equation is a constitutive relation between the flux $\mathbf{q}_i$ and the gradient of temperature T^i. The parameter λ_i is a scalar type conductivity coefficient. Equations (3) and (4) are applicable to the both phases, and the index i is defined as

$$i = \begin{cases} c, & \text{for the continuous phase} \\ d, & \text{for the dispersed phase.} \end{cases} \tag{5}$$

The index i appears as a subscript at all quantities except temperature T, where it is used in the form of a superscript. The boundary conditions at the cylinder surface $r = a$ (where $a = b/l$) are as follows:

$$T^c = T^d \tag{6}$$

$$\lambda_c \frac{\partial T^c}{\partial r} = \lambda_d \frac{\partial T^d}{\partial r}. \tag{7}$$

These equations result from the assumed continuity of the temperature T and the heat flux $\mathbf{q}$ at $r = a$. Besides the boundary conditions (6) and (7) at the cylinder surface, one further condition at the external border of the cell is required. This condition results from the periodicity of the solution, and is equivalent to the known Rayleigh identity [4]. We shall return to this condition later.

The volume fraction of the dispersed phase φ is related to the cylinder radius by

$$\varphi = \frac{V_d}{V} = \frac{\pi b^2}{l^2} = \pi a^2. \tag{8}$$

The limiting volume fraction corresponding to the touching cylinders ($b = l/2$) is

$$\varphi_{\max} = \pi/4 \tag{9}$$

for the square array. It is often convenient to introduce the ratio

$$f = \frac{\varphi}{\varphi_{\max}} = 4a^2 \tag{10}$$

instead of φ. Throughout this paper we shall use both φ (9) and f (10) alternatively.

The array has a form of a simply connected region Ω. If the length l is sufficiently small compared to the macroscopic length scale L of the region Ω, then the composite may be treated as homogeneous from the macroscopic point of view. Its bulk properties may be expressed by the effective conductivity coefficient, λ_{ef}, defined by the relation

$$\langle \mathbf{q} \rangle = -\lambda_{\text{ef}} \cdot \langle \nabla T \rangle. \tag{11}$$

Here $\langle \mathbf{q} \rangle$ and $\langle \nabla T \rangle$ denote the volume-averaged heat flux and the volume-averaged temperature gradient, respectively. We shall return to the problem of calculating λ_{ef} in Section 3.

In the case when $l \ll L$ the potential T^i inside the region Ω may be well approximated by the sum

$$T^i = T_M + T^i_P, \tag{12}$$

where T_M is a macroscopic and T^i_P is a periodic microscopic component. The component T_M depends on the shape of Ω whereas T^i_P is independent of the shape of Ω and depends on the geometrical structure and physical properties of the array. In the thermodynamic limit when $\Omega \to \infty$ or $l \to 0$ the relation (12) holds exactly [11, 12].

In this paper we consider the case where a uniform macroscopic temperature gradient, $\mathbf{G}_0$, is imposed upon the composite material in the x-direction. A uniform temperature gradient corresponds to the elliptical shape of the region Ω. However, for other shapes considering a locally uniform temperature gradient is a good approximation, provided $l \ll L$. We may then present the relation (12) in the form

$$T^i = G_0 x + T^i_P, \tag{13}$$

where G_0 is the x-component of the gradient vector $\mathbf{G}_0$, the y-component being equal to zero.

The periodic component T^i_P can be calculated with the aid of the method which is sometimes called the induced sources method, and was previously applied to composites with spherical inclusions arranged in cubic arrays [9, 10]. In this method we first search for a periodic solution T^c_P in a continuous phase. With this aim we consider the composite as consisting of a matrix material in which the inclusions are replaced by singular multipole source distributions located at their centres $\mathbf{R}_n$. On the basis of the above assumption we can insert equation (13) into (3) and (4) and obtain the Poisson equation for T^c_P

$$\lambda_c \nabla^2 T^c_P = -\rho_c. \tag{14}$$

The distribution of singular sources ρ_c is given in ref. [9] presented with the aid of generalized functions. Sangani and Acrivos [10] presented the solution of (14) in the form

$$T^c_P = \mathscr{D} T_0, \tag{15}$$

where $\mathscr{D}$ is a differential operator and T_0 corresponds to a Wigner potential [11]. Sangani and Acrivos found the solution for the regular three-dimensional composite with the spherical inclusions.

In the two-dimensional case the form of $\mathscr{D}$ given in [10] is as follows:

$$\mathscr{D} = \sum_{k=1}^{\infty} P_k \frac{\partial^k}{\partial x^k}, \tag{16}$$

where P_k are unknown coefficients. Sangani and Acrivos [10] confined themselves to the presentation of (16) without making further calculations. These calculations are carried out here using the two-dimensional Wigner potential, given in ref. [12]

$$T_0 = -\ln r + \tfrac{1}{2}\pi r^2 + \sum_{m=1}^{\infty} A_m r^m \cos m\theta. \quad (17)$$

The potential (17) is periodic by definition, hence the coefficients A_m must be chosen such that the condition

$$\mathbf{n}\cdot\nabla T_0 = 0 \quad (18)$$

should be fulfilled at the cell boundary. The coefficients A_m may be expressed as sums over an infinite array and evaluated by the Evald method [11, 12]. With respect to the symmetry of the square array these coefficients are different from zero only for m which are multiples of 4. Numerical values of the coefficients A_m are given in ref. [12] for several values of m.

The coefficients A_m are related to the coefficients S_m used by Rayleigh [4] with the aid of the following equality [13]:

$$A_m = \frac{S_m}{m}. \quad (19)$$

Numerical values of S_m for the square array are given in ref. [6].

Based on equations (15)–(17) we can present the periodic component T_P^c of the temperature in the continuous phase in the form of the following expansion:

$$T_P^c = \sum_{k=1}^{\infty} P_k T_k^c, \quad (20)$$

where T_k^c denotes functions obtained by subsequent derivation of T_0 (15):

$$T_k^c = (-1)^k (k-1)! \frac{\cos k\theta}{r^k} + \pi(\delta_{1k} r\cos\theta + \delta_{2k}) + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} A_{k+m} r^m \cos m\theta. \quad (21)$$

The periodic component T_P^d of temperature in the dispersed phase can be presented as

$$T_P^d = \sum_{k=1}^{\infty} Q_k T_k^d, \quad (22)$$

where the functions T_k^d, nonsingular at $r = 0$, have the form

$$T_k^d = (-1)^k (k-1)! \frac{r^k}{a^{2k}} \cos k\theta + \pi(\delta_{1k} r\cos\theta + \delta_{2k}) + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} A_{k+m} r^m \cos m\theta, \quad (23)$$

and Q_k are unknown coefficients. The basic functions $T_k^c(r,\theta)$ and $T_k^d(r,\theta)$ have been first derived and discussed in ref. [13]. The periodicity condition is fulfilled identically here owing to the periodic properties of the Wigner potential (18) involved in the derivation of the basic functions (21), (23). The lack of singularity of the solution at $r = 0$ follows from equation (23). From the condition (6) we get immediately

$$P_k = Q_k. \quad (24)$$

With respect to the symmetry conditions for the square array these coefficients are equal to 0 for even k.

The unknown coefficients, P_k, have to be determined from the boundary condition (7). Inserting equation (13) to (7) and taking $x = r\cos\theta$ we get

$$\frac{1}{2\alpha}\frac{\partial}{\partial r}(T_P^c - T_P^d) + \frac{1}{2}\frac{\partial}{\partial r}(T_P^c + T_P^d) = -G_0 \cos\theta, \quad (25)$$

where

$$\alpha = \frac{1-h}{1+h}. \quad (26)$$

Now let us substitute equations (20) and (22) with (21) and (23) in (25) and collect terms with respect to $\cos k\theta$. After differentiation and some rearrangements one then obtains the following system of equations

$$\left(\frac{1}{\alpha}\hat{I} - \hat{Z}\right)\mathbf{X} = \mathbf{D}, \quad (27)$$

where $\mathbf{D}$ is a column vector whose first element is 1 and all the others are equal to 0, $\hat{I}$ is the unit matrix and $\hat{Z}$ is a symmetric matrix.

The unknown vector $\mathbf{X}$ has its elements related to P_k by (28)

$$X_{2n-1} = -\frac{\sqrt{2n-1}}{G_0 a^{2n}} (2n-2)!\, P_{2n-1} \quad (28)$$

and the elements of the matrix $\hat{Z}$ have the following form:

$$Z_{mn} = -\varphi\delta_{1m}\delta_{1n} + W_{mn} \quad (29)$$

$$W_{mn} = -\frac{(2m+2n-2)!\, A_{2m+2n-2}}{4^{m+n-1}(2m-2)!\,(2n-2)!\sqrt{2m-1}\sqrt{2n-1}} \times f^{m+n-1}, \quad m,n = 1,2,\ldots, \quad (30)$$

where φ and f are related by (10). The system of equations (27) together with (29) and (30) involves two parameters: α (26) and the volume fraction of the dispersed phase φ (or f). With the aid of the relations (28), (13), (20) and (22) the solution of (27) allows one to calculate temperature distribution in the continuous as well as in the dispersed phase.

3. THE EFFECTIVE TRANSPORT COEFFICIENT

Now we rederive the Rayleigh formula [4] for the effective transport coefficient (11) in the case of the square array of cylinders. With this aim we evaluate the volume-averaged quantities which may be expressed as

$$\langle F\rangle = (1-\varphi)\langle F_c\rangle + \varphi\langle F_d\rangle, \quad (31)$$

where F is any given function of the position, and the average quantities $\langle F_i\rangle$ are defined as

$$\langle F_i\rangle = \frac{1}{V_i}\int_{V_i} F_i \,\mathrm{d}v \quad (32)$$

in each phase, V_i being the volume of the ith phase. With the aid of (4) we apply (31) to the heat flux and the temperature gradient. Thus we obtain

$$\langle \mathbf{q}\rangle = -(\lambda_c(1-\varphi)\langle \nabla T^c\rangle + \lambda_d\varphi\langle \nabla T^d\rangle) \quad (33)$$

$$\langle \nabla T\rangle = G_0 = (1-\varphi)\langle \nabla T^c\rangle + \varphi\langle \nabla T^d\rangle. \quad (34)$$

Substituting (33) and (34) into (11) upon some rearrangement we get the following formula for the effective coefficient:

$$\mu = \frac{\lambda_{\mathrm{ef}}}{\lambda_c} = 1-(1-h)\frac{\varphi\langle \nabla T^d\rangle}{G_0}. \quad (35)$$

The mean temperature gradient in the dispersed phase $\langle \nabla T^d\rangle$ can be calculated from (32) with the aid of (22)–(24) by integration of the temperature field in a unit cell:

$$\langle \nabla T^d\rangle = -\frac{2P_1}{(1-h)a^2}. \quad (36)$$

Substituting equation (36) into (35), we obtain the following formula for the effective conductivity coefficient:

$$\mu = 1+2\pi\frac{P_1}{G_0}. \quad (37)$$

Since we intend to search for the solution of our problem with the aid of equation (27), we replace B_1 in (37) by X_1 (28) and get a new form of relation (27):

$$\mu = 1-2\varphi X_1. \quad (38)$$

Now we can easily derive the effective conductivity coefficient in its first approximation solving equation (27) for $m = n = 1$. In this case (27) takes the form

$$\left(\frac{1}{\alpha}+\varphi\right)X_1 = 1 \quad (39)$$

and (38) yields

$$\mu = 1-\frac{2\alpha\varphi}{\alpha\varphi+1}. \quad (40)$$

These calculations were first carried out by Maxwell [3] but the corresponding formula (40) has the form derived later by Garnett. The relation (40), known in the literature as the Maxwell–Garnett formula, is equivalent to the earlier Clausius–Mosotti formula for the dielectric constant. It does not depend on the detailed geometric structure of the composite: however, it is valid in a rather limited range of parameters α, φ.

4. METHOD OF SOLUTION

As follows from (38), the effective transport coefficient depends only on the first component X_1 of the solution of (27). It can be written formally as

$$X_1 = \frac{\left|\frac{1}{\alpha}\hat{I}^S - \hat{Z}^S\right|}{\left|\frac{1}{\alpha}\hat{I} - \hat{Z}\right|}, \quad (41)$$

where a matrix with the superscript S denotes a submatrix of the original matrix, corresponding to its first element. The coefficients W_{mn} (30) define the matrix $\hat{W}$; and it is seen from equation (29) that

$$\hat{Z}^S = \hat{W}^S. \quad (42)$$

Now we shall put the relation (41) into a more advantageous form. The Wigner coefficients $A_{2(m+n-1)}$ are different from 0 for odd $m+n$. As a consequence the nonzero elements W_{mn} (30) of the matrix ($\hat{W}$) depend on even powers of φ. However, it is seen from (29) that the first element of the matrix $\hat{Z}$ is linear with respect to φ

$$Z_{11} = -\varphi. \quad (43)$$

With the aid of the identity

$$\left|\frac{1}{\alpha}\hat{I}-\hat{Z}\right| = \left|\frac{1}{\alpha}\hat{I}-\hat{W}\right| + \varphi\cdot\left|\frac{1}{\alpha}\hat{I}^S-\hat{W}^S\right| \quad (44)$$

which follows directly from (29), we separate the term linear with respect to φ, and replace in our considerations the matrix $\hat{Z}$ by the matrix $\hat{W}$, thus preserving merely terms depending on even powers of φ. Inserting equation (44) into (41) and denoting

$$Y_1 = \frac{\left|\frac{1}{\alpha}\hat{I}^S - \hat{W}^S\right|}{\left|\frac{1}{\alpha}\hat{I} - \hat{W}\right|}, \quad (45)$$

we get the relation between X_1 and Y_1

$$X_1 = \frac{1}{\varphi+1/Y_1}. \quad (46)$$

Multiplying the numerator and denominator of the fraction (46) by α and inserting it into the formula (38) we get

$$\mu = 1-\frac{2\alpha\varphi}{\alpha\varphi+\alpha/Y_1}. \quad (47)$$

Substituting for the ratio φ/Y_1 a new parameter β

$$\beta = \alpha/Y_1 \quad (48)$$

we obtain the following general formula for the effective transport coefficient:

$$\mu = 1-\frac{2\alpha\varphi}{\alpha\varphi+\beta}. \quad (49)$$

This formula closely resembles the Maxwell–Garnett formula (40) except that here we have β instead of 1. It will be seen from the following that β is a more convenient form for representing the effective transport coefficient than μ. The parameter β is related to Y_1 and may be obtained by solving the system (50), whose coefficients depend on even powers of f:

$$\left(\frac{1}{\alpha}\hat{I}-\hat{W}\right)\mathbf{Y}=\mathbf{D}. \tag{50}$$

The solution of (50) may be represented in the form

$$\mathbf{Y}=\left(\frac{1}{\alpha}\hat{I}-\hat{W}\right)^{-1}\mathbf{D}. \tag{51}$$

Making use of the identity

$$(\hat{I}-\alpha\hat{W})^{-1}=\sum_{n=0}^{\infty}\alpha^n\hat{W}^n \tag{52}$$

and remembering that $Y_1=\alpha/\beta$, and the only nonzero component of $\mathbf{D}$ is D_1 ($D_1=1$) we obtain from (51)

$$\frac{1}{\beta}=\sum_{n=0}^{\infty}\alpha^n(\hat{W}^n)_{1,1}. \tag{53}$$

The matrix $\hat{W}$ (30) has the chess-board type structure: the matrix elements with the even sum of indices are equal to 0. This structure of zero elements remains unchanged for the odd powers of the matrix; in particular

$$(\hat{W}^{2k-1})_{1,1}=0,\quad \text{for } k=1,2,\ldots. \tag{54}$$

It follows from equations (53) and (54) that β depends on α^2. This result is equivalent to the Keller symmetry [18].

The elements of the matrix $\hat{W}$ with the odd sum of indices are proportional to the even positive powers of f, the lowest exponent of f being 2. The nonzero elements of the matrix $\hat{W}^2$ are the products of rows and columns of the matrix $\hat{W}$, and therefore have the form of power series of f^4, with the lowest exponent of f being 4. As a consequence of the fact that all nonzero elements of $\hat{W}$ are the positive powers of f^2, the lowest exponent of f in the elements of powers of the matrix $\hat{W}$ increases with the matrix exponent, and equals $4k$ for $\hat{W}^{2k}$. Thus we obtain

$$\frac{1}{\beta}=\sum_{k=0}^{\infty}c_k\alpha^{2k}=\sum_{k=0}^{\infty}\left(\alpha^{2k}\left(\sum_{j=k}^{\infty}c_{kj}f^{4j}\right)\right). \tag{55}$$

The coefficients c_{kj} may be calculated numerically from equations (53) and (27).

5. REPRESENTATION OF β BY A CONTINUED FRACTION

The power series is not a reasonable form for representing β. As was stated in the Introduction, the effective conductivity coefficient as a function of the complex argument h (for the given geometrical structure) is a Stieltjes function: this means that it has poles of the first order on the real negative semi-axis. The location of the poles restricts the convergence radius of the power series. Taking as the argument α, instead of h, we obtain as a physically meaningful range $|\alpha|\leqslant 1$, while the negative values of h correspond to $|\alpha|>1$. In this case the physically meaningful range lies inside the convergence circle. But even in this case, the poles lying near $|\alpha|=1$ make the power series converge very slowly. The continued fraction, whose subsequent approximants are rational functions, is much better adapted to represent such functions. It should be taken into account that the poles of the functions $\mu(\alpha)$ or $\beta(\alpha^2)$ lie, in any case partially, on the positive semi-axis. In this case the corresponding series are not the Stieltjes series, but their generalized form—the Hamburger series. However, even in this case using the continued fraction is very fruitful.

The power series (55) may be represented as a J-fraction [15] of the argument $1/\alpha^2$, the coefficients of the fraction being power series of f^4. This transformation may be done numerically with the aid of the algorithm presented in ref. [15]. Similarly to equation (55), the lowest power of f in the power series representing the coefficients of subsequent levels of the continued fraction increase with the order of the level, but this growth is even larger than in equation (55). In the following, we present argumentation which makes possible to determine the lowest powers of f for the coefficients of the J-fraction for $\beta(1/\alpha^2)$. Since the full calculations are rather complicated, we shall give only their brief outline. First let us write two expressions for $1/\beta$; the first one follows directly from (45) and (48):

$$\frac{1}{\beta}=\frac{1}{\alpha}\cdot\frac{\left|\frac{1}{\alpha}\hat{I}^S-\hat{W}^S\right|}{\left|\frac{1}{\alpha}\hat{I}-\hat{W}\right|}, \tag{56}$$

while the second is the expansion of the power series (55) into an S-fraction [15]:

$$\frac{1}{\beta}=\frac{1}{1}-\frac{k_1}{1/\alpha^2-}\frac{k_2}{1-}\frac{k_3}{1/\alpha^2-}\frac{k_2}{1-}\cdots. \tag{57}$$

The nth approximant of the continued fraction (57) may be presented as a rational function of $1/\alpha^2$. In a similar way we may express $1/\beta$ from (56), upon truncating the matrices $\hat{I}$ and $\hat{W}$ to n rows and n columns. We obtain

$$\frac{1}{\beta}=\left(\sum_{i=0}^{m}p_i^{(j)}\alpha^{-2i}\right)\Big/\left(\sum_{i=0}^{m}q_i^{(j)}\alpha^{-2i}\right), \tag{58}$$

where $m=$ entier $(n/2)$ and $j=1,2$ for the rational functions obtained from (57) and (56), respectively. Transforming the continued fraction (57) to a rational function involves only four fundamental arithmetical operations, so the coefficients $p_i^{(j)}$ and $q_i^{(j)}$ of the rational function are certain polynomials of $k_1,k_2,\ldots,k_n$. These polynomials have a particularly simple form for $p_0^{(1)}$ and $q_0^{(1)}$:

$$p_0^{(1)} = -k_2 \cdot k_4 \ldots k_{2m}, \qquad \text{for } n = 2m+1$$

$$q_0^{(1)} = -k_1 \cdot k_3 \cdots k_{2m-1}, \quad \text{for } n = 2m. \qquad (59)$$

It follows from (56) and (58) that $p_0^{(2)}$ and $q_0^{(2)}$ are equal to $|\hat{W}^S|$ and $|\hat{W}|$, respectively. Each term of the determinant of the order k is a product of k matrix elements. The sum of all $2k$ indices in each product is the same and equals $k(k+1)$. The nonzero elements of the matrix $\hat{W}$ are powers of f (30) with the exponents determined by the sum of indices of the element. Consequently, each term of the determinant is proportional to f with the same exponent, and the nonzero determinants of $\hat{W}$ are powers of f. It results from (30) that upon truncation of the matrix $\hat{W}$ to n columns and n rows, $|\hat{W}|$ is equal to 0 for odd n and is proportional to f^{n^4} for even n; on the other side $|\hat{W}^S|$ is equal to 0 for even n and is proportional to f^{n^2-1} for odd n. We then obtain

$$p_0^{(2)} = |\hat{W}^S| = \text{const} \cdot f^{4m(m+1)}, \quad \text{for } n = 2m+1$$

$$q_0^{(2)} = |\hat{W}| = \text{const} \cdot f^{4m^2}, \qquad \text{for } n = 2m. \qquad (60)$$

The coefficients c_k in (55) are power series of f^4. The same is valid for the coefficients k_i, because the corresponding transformation from c_i to k_i only involves arithmetical operations

$$k_i = \sum_j k_{ij} f^{4j}, \quad i = 1, \ldots, n. \qquad (61)$$

Now let us see what is the lowest power of f in (61). We denote by k_i^0 the term with the lowest power of f within k_i. In general, the values of k_{ij} depend on the size of the matrix ($n \times n$). However, it appears that the values of k_i^0 do not depend on n. Comparing $q_0^{(1)}$ with $q_0^{(2)}$ or $p_0^{(1)}$ with $p_0^{(2)}$ we obtain two forms of equations for the coefficients k_i for n even and odd, respectively

$$k_2 \cdot k_4 \cdots k_{2m} = \text{const} \cdot f^{4m(m+1)}, \quad \text{for } n = 2m$$

$$k_1 \cdot k_3 \cdots k_{2m-1} = \text{const} \cdot f^{4m^2}, \quad \text{for } n = 2m+1. \quad (62)$$

In accordance with equations (62), the products of the power series k_i are power functions with integer exponent. Since in the multiplication of power series the product of terms with the lowest exponents cannot be cancelled, we have

$$k_2^0 \cdot k_4^0 \cdots k_{2m}^0 = \text{const} \cdot f^{4m(m+1)}, \quad \text{for } n = 2m$$

$$k_1^0 \cdot k_3^0 \cdots k_{2m-1}^0 = \text{const} \cdot f^{4m^2}, \qquad \text{for } n = 2m+1. \qquad (63)$$

We have obtained the recurrent system of equations (63) for any given n. Solving this system we simply find that the lowest power of f within k_i is $4i$:

$$k_i^0 = \text{const} \cdot f^{4i}, \quad i = 1, 2, \ldots. \qquad (64)$$

The S-fraction (57) can be transformed to a J-fraction ([15], chapter 4.5)

$$\beta = 1 - \frac{K_1}{L_1 + (1/\alpha^2) -} \frac{K_2}{L_2 + (1/\alpha^2) -} \cdots, \qquad (65)$$

where

$$K_1 = k_1, \qquad L_1 = -k_2,$$

$$K_j = k_{2j-2} \cdot k_{2j-1}, \quad L_j = -(k_{2j-1} + k_{2j}),$$

$$j = 2, 3, \ldots. \qquad (66)$$

Making use of (66) we may present the coefficients of the continuous fraction (65) in the form of power series of f^4:

$$K_n = f^{4(4n-3)} \sum_{j=0}^{\infty} K_{nj} f^{4j}$$

$$L_n = f^{4(2n-1+\delta_{1n})} \sum_{j=0}^{\infty} L_{nj} f^{4j}, \quad n = 1, 2, \ldots. \quad (67)$$

6. NUMERICAL RESULTS

In the previous section we gave the expression for β in the form of a J-fraction with the argument $1/\alpha^2$, the coefficients of which have the form of power series with the argument f^4. If f is not too close to 1, then the coefficients K_n rapidly decrease and only very few levels of the fraction (65) have an influence on the value of the fraction (see Fig. 2).

However, if f becomes near to 1, the formula (67) becomes less convenient: the coefficients K_{nj} and L_{nj} of the power series in (67) decrease slowly with j for $n > 1$ (for low j they may even increase). The number of these coefficients needed for evaluation of K_n, L_n for a given f near to 1 may be much greater than the number of necessary levels of the continued fraction. In this case a more tractable expression for β may be obtained by replacing the power series (67) by their Padé approximants [19]. Taking into account $4M$ as the highest power of f we have

$$K_n = f^{16(n-1)} \frac{\sum_{j=1}^{M} s_{nj} f^{4j}}{1 + \sum_{j=1}^{M} S_{nj} f^{4j}}$$

$$L_n = f^{8(n-1)+4\delta_{1n}} \frac{\sum_{j=1}^{M} t_{nj} f^{4j}}{1 + \sum_{j=1}^{M} T_{nj} f^{4j}}. \qquad (68)$$

An algorithm calculating the coefficients s_{nj}, S_{nj}, t_{nj}, T_{nj} has been obtained. The algorithm enables calculations for arbitrary number of fraction levels and arbitrary M within the limits of computer memory. In Table 1 we have limited ourselves to the coefficients for $n = 1$, 2 and $j = 1, \ldots, 4$, because further increasing of the coefficients' number furnish only a little progress in accuracy near the singular point. For $n = 1$ the power series representation (67) is used, thus the coefficients S_{1j} and T_{1j} being equal to zero.

Table 1. Coefficients of the continuous fraction for β

n	j	s_{nj}	S_{nj}	t_{nj}	T_{nj}
1	1	0.11637	0.00000	−0.20313	0.00000
	2	0.00193	0.00000	−0.05203	0.00000
	3	0.00000	0.00000	−0.01178	0.00000
	4	0.00000	0.00000	−0.00317	0.00000
2	1	0.02046	−1.33165	−0.10072	−1.56126
	2	−0.01181	0.60125	0.03172	0.95059
	3	0.00223	−0.07218	0.01770	−0.28559
	4	−0.00030	−0.02059	−0.01764	0.03875

The formulae (68) together with Table 1 accurately determine the effective conductivity coefficient in all the range of α and f, except the neighbourhood of the singular point at $\alpha^2 = 1$ and $f = 1$, where the asymptotic formula, known from the literature [7] should be applied. The accuracy of (68) as compared with the formulae of other authors is presented in Fig. 2. In the figure the lines bounding the regions in which accuracy of particular formulae are better than 1% are drawn. The region of applicability of a particular formula lies underneath the drawn line. It is seen that the formula (49) together with (65) and (68) has the largest region of applicability.

Another representation of the effective transport coefficient is the representation by poles. Because the function $\mu(h)$ is a Stieltjes functions, its poles lay on the negative real semi-axis in the complex h-plane. It is convenient to consider the poles of $\beta(\alpha^2)$ instead of $\mu(h)$ because each pole of $\beta(\alpha^2)$ corresponds to two poles of $\mu(h)$ for $h = (1+\alpha)/(1-\alpha)$ and $h = (1-\alpha)/(1+\alpha)$, respectively:

$$\beta = 1-\sum_k \frac{\text{res}_k}{\alpha^2-\text{arg}_k}. \tag{69}$$

In this case the main pole corresponding to the Maxwell–Garnett formula is absent. The poles of $\beta(\alpha^2)$ are located in the infinite interval $(1, \infty)$ of α^2. The locations and values of residua of three first poles of $\beta(\alpha^2)$ are shown in Fig. 3, where arg means $1/\alpha^2$ and res represents the value of the residuum. However, it should be noted that the representation by means of continued fraction is more advantageous than the representation by poles. It follows from the fact that the knowledge of the several first coefficients of the continued fraction enables the evaluation of the first moments of the spectral density function. This is not possible in the case of the representation by poles.

7. CONCLUSIONS

In this paper a recursion method has been derived to obtain the effective conductivity coefficient of a composite as a continued fraction representation for α, with fraction coefficients being functions of f. This method was applied to a square array of cylinders embedded in a homogeneous matrix: however, the method has a more general character and may be applied to other regular arrays of cylinders or spheres. The obtained formula in a form of a continued fraction provides rapid convergence, and it appears that two levels of the fraction are sufficient to get a good accuracy in a wide range of parameters. Together with the asymptotic formula [7] it covers the full range of parameters. Analysis of the quantity β, which appears in the expression (49) for μ, is more convenient than the direct analysis of $\mu(\alpha, f)$, because β reveals a higher degree of symmetry as a function of parameters: $\beta = \beta(\alpha^2, f^4)$.

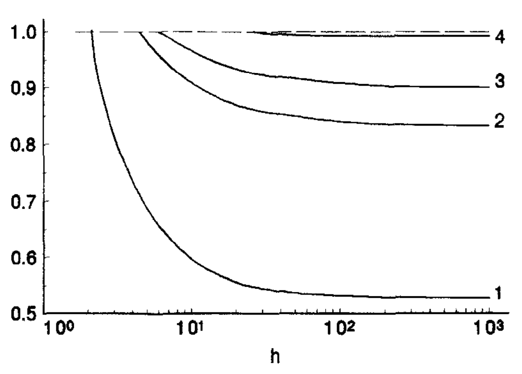

FIG. 2. Upper bound of regions of applicability (error < 1%) of the formulae for the effective conductivity coefficient: (1) Maxwell–Garnett, (2) Rayleigh, (3) McPhedran et al., (4) present results.

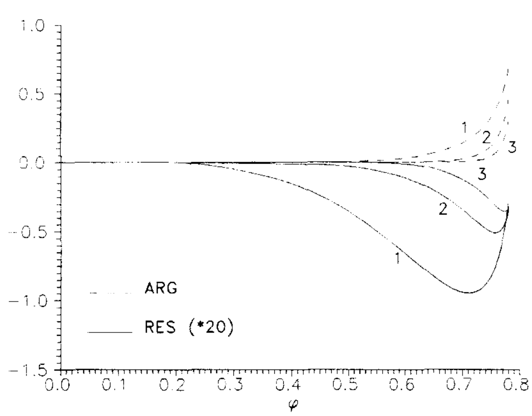

FIG. 3. The arguments and residua of the first three poles of the function $\beta(\alpha^2)$.

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