Arch. Mech., 2, pp. 319–327, Warszawa 2000

Brief Notes

Quasifractional approximants for effective conductivity of regular arrays of spheres (1)

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We study the effective heat conductivity of regular arrays of perfectly conducting spheres embedded in a matrix with the unit conductivity. Quasifractional approximants allow us to derive an approximate analytical solution, valid for all values of the spheres volume fraction $\varphi \in [0; \varphi_{\max}]$ ($\varphi_{\max}$ is the maximum limiting volume of a sphere). As the bases we use a perturbation approach for $\varphi \to 0$ and an asymptotic solution for $\varphi \to \varphi_{\max}$. Three different types of the spheres space arrangement (simple, body and face-centred cubic arrays) are considered. The obtained results give a good agreement with numerical data.

1. Introduction

One of the main tasks of the theory of dispersed media is a theoretical prediction of effective transport properties. The problem could be formulated in a number of mathematically equivalent ways, but here we shall discuss it in the language

(1) The main results of this paper were presented at the 32nd Solid Mechanics Conference (Zakopane, 1998) [12, 13].

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of heat conductivity: we wish to determine the effective heat conductivity k of infinite regular arrays of identical, perfectly conducting spheres of the volume fraction φ, embedded in an isotropic matrix with the unit conductivity.

BATCHELOR [1] displayed a number of light distinct physical problems which can be solved by analogous mathematical methods. One of these is the above mentioned conductivity problem, while others involve calculating the dielectric constant, the magnetic permeability, the electric conductivity, elastic constants, etc. Thus, prediction of the effective conductivity of a two-phase medium spans many fields, and a great deal of efforts have been devoted to its resolution. Therefore, we can not possibly summarise even a small fraction of the previous investigations of the subject. A detailed review can be found, for example, in ref. [1]. Here we shall give a brief account of those papers of direct relevance to our work.

The calculation of k for general types of composites was originally discussed by J. C. MAXWELL [2], and subsequently has been considered by many others. The solution for the case of small spheres (φ tends to zero) was first examined by Lord RAYLEIGH [3], who described the polarization of each sphere in an external field by an infinite set of multipole moments. This method has recently been extended, with the aid of modern digital computers, so that a large number of multipoles can now be calculated [4, 5].

In the case of large, nearly touching spheres (φ tends to its maximum limiting value $\varphi_{\max}$), KELLER [6] derived an asymptotic solution of the problem. His work was extended by BATCHELOR and O'BRIEN [7] and by VAN TUYL [8]. However, there still remains a certain parameter range which is covered neither by the asymptotic approach nor by the solution based on the assumption of small φ.

Practically any physical or mechanical problem, which includes a variable parameter, can be approximately solved as this parameter approaches zero or infinity. How can this "limiting" information be used in the study of the system at the intermittent values of the parameter? This problem is one of the most complicated ones in asymptotic analysis. In many instances the answer to it is alleviated by two-point Padé approximants [9]. Some effective applications of two-point Padé approximants to the theory of dispersed media can be found in [10].

Unfortunately, the asymptotic formula for $\varphi \to \varphi_{\max}$ contains the logarithmic function; that is why two-point Padé approximants in its "pure form" can not be used in the problem under consideration. This point is most essential for two-point Padé approximants because, as a rule, one of the limits ($\lambda \to 0$ or $\lambda \to \infty$) for real mechanical problems gives expansions with logarithmic terms or other complicated functions. In order to overcome these obstacles, during the last few years the so-called quasifractional approximants are widely used in physics [11].

Here we use quasifractional approximants to derive an approximate analytical expression of k, valid for all values of the spheres volume fraction $\varphi \in [0; \varphi_{\max}]$

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[12, 13]. As the bases we use the coefficients of the perturbation expansion of k at $\varphi = 0$ and the asymptotic formula for $\varphi \to \varphi_{\max}$. Three different types of the spheres space arrangement (simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC) arrays) are considered. The obtained results give a good agreement with numerical data.

This paper is organized as follows: in Sec. 2 and in Sec. 3 we define the "limiting" solutions for $\varphi \to 0$ and for $\varphi \to \varphi_{\max}$. The quasifractional approximant is developed in Sec. 4. In Sec. 5 the obtained results are compared with known numerical data, and in Sec. 6 we discuss the advantages and limitations of our method.

2. Solution for the case of small spheres

Lord RAYLEIGH [3] was the first to analyze the case when spheres are arranged in the SC array. He developed a solution for the case $\varphi \to 0$ by replacing the spheres by dipoles and higher-order multipoles, and obtained

$$k = 1 - 3\varphi \left(\frac{2+\lambda}{1-\lambda} + \varphi - \frac{1-\lambda}{4+3\lambda} d\varphi^{10/3} + O\left(\varphi^{14/3}\right)\right)^{-1}, \tag{2.1}$$

where φ is the spheres volume fraction; λ is the heat conductivity of spheres; $d = 1.57$.

MEREDITH and TOBIAS [14] extended Rayleigh's analysis and calculated the coefficient of the $O(\varphi^{14/3})$ term. The validity of Rayleigh's method, however, was questioned, because it involves the summation of non-absolutely convergent series. MCPHEDRAN and MCKENZIE [4] have modified Rayleigh's procedure in order to overcome these difficulties and, hence, this method has now a sound theoretical basis.

An alternative method, which avoids the difficulties encountered in Rayleigh's original treatment, was devised by ZUZOVSKY and BRENNER [15]. They used the method of generalized functions to develop a series expression for k to $O(\varphi^{20/3})$ and found that the coefficient of $O(\varphi^{14/3})$ in (2.1) reported by MEREDITH and TOBIAS [14] was in error. But, owing to a numerical slip in calculations, some results of Zuzovsky and Brenner were incorrect. The next development of this method was carried out by SANGANI and ACRIVOS [5], who corrected the previous errors and obtained the following perturbation expansion for k in terms of φ:

$$k = 1 - 3\varphi \left(-\frac{1}{L_1} + \varphi + a_1 L_2 \varphi^{10/3} \frac{1 + a_2 L_3 \varphi^{11/3}}{1 - a_3 L_2 \varphi^{7/3}} + a_4 L_3 \varphi^{14/3} + a_5 L_4 \varphi^6 + a_6 L_5 \varphi^{22/3} + O(\varphi^{25/3})\right)^{-1}, \tag{2.2}$$

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where $L_i = \dfrac{\lambda - 1}{\lambda + 2i/(2i-1)}$, $i \in N$ (here we consider the case of perfectly conducting spheres, $\lambda = \infty$; $L_i = 1$); the constants $a_1, ..., a_6$ for the three cubic arrays are listed in Table 1.

Table 1. The constants $a_1, ..., a_6$.

	a_1	a_2	a_3	a_4	a_5	a_6
SC array	1.305	0.231	0.405	0.0723	0.153	0.0105
BCC array	0.129	−0.413	0.764	0.257	0.0113	0.00562
FCC array	0.0753	0.697	−0.741	0.0420	0.0231	$9.14 \cdot 10^{-7}$

It should be stressed that further development of this method by taking into account the terms of higher order in the perturbation expansion (2.2), however, does not allow us to calculate k correctly in the case of large spheres ($\varphi \to \varphi_{\max}$).

3. Solution for the case of large spheres

In the case of perfectly conducting large spheres ($\lambda = \infty, \varphi \to \varphi_{\max}$), the problem can be solved by means of a reasonable physical assumption that the flux of heat occurs entirely in the region where spheres are in near contact. Thus, the effective conductivity is determined in an asymptotic form for the flux between two spheres, which is logarithmically singular in the gap width, justifying the assumption. KELLER [6] solved this problem correctly to $O(\ln \chi)$, where χ is the dimensionless gap width ($\chi \to 0$). BATCHELOR and O'BRIEN [7] extended Keller's work to include touching spheres and near-perfect conductors, and derived the following asymptotic expansion for $\lambda = \infty$ and $\varphi \to \varphi_{\max}$:

$$k = -M_1 \ln \chi - M_2 + O(\chi^{-1}), \tag{3.1}$$

where $\chi = 1 - (\varphi/\varphi_{\max})^{1/3}$ is the nondimensional gap width between the neighbouring spheres, $\chi \to 0$; $M_1 = 0.5\varphi_{\max} p$, p is the number of contact points at the surface of a sphere; M_2 is a constant, dependent on the type of spheres space arrangement. The values of M_1, M_2 and $\varphi_{\max}$ for the three cubic arrays are listed in Table 2.

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Table 2. The constants M_1, M_2 and $\varphi_{\max}$.

	M_1	M_2	$\varphi_{\max}$
SC array	$\pi/2$	0.7	$\pi/6$
BCC array	$\sqrt{3}\pi/2$	2.4	$\sqrt{3}\pi/8$
FCC array	$\sqrt{2}\pi$	7.1	$\sqrt{2}\pi/6$

VAN TUYL [8] has recently calculated the next higher order terms in the asymptotic expansion (3.1).

4. The quasifractional approximant

Now we go on to the problem of evaluating the effective conductivity k in terms of the quasifractional approximants [11, 12]. So, we consider a function of φ determined by the power series expansion (2.2) at $\varphi \to 0$ and knowing the asymptotic expansion (3.1) at $\varphi \to \varphi_{\max}$. A singularity of the searching solution involves the logarithmic function in the expression (3.1). In order to reproduce this singularity, the quasifractional approximant has to contain a similar term, so it can be written as follows:

$$k = \left(P_1(\varphi) + P_2\varphi^{(m+1)/3} + P_3 \ln \chi\right)/Q(\varphi), \tag{4.1}$$

where rational functions $P_1(\varphi)$, $Q(\varphi)$ and constants P_2, P_3 are determined from the following conditions: (i) the expansion of (4.1) in powers of φ at $\varphi \to 0$ coincides with m leading terms of the perturbation expansion (2.2), and (ii) the asymptotic behaviour of (4.1) at $\varphi \to \varphi_{\max}$ coincides with n leading terms of the asymptotic expansion (3.1). Thus, we obtain:

$$Q(\varphi) = 1 - \varphi - a_1\varphi^{10/3}; \qquad P_1(\varphi) = \sum_{i=0}^{m} \alpha_i \varphi^{i/3};$$

$$P_2 = \begin{cases} 0, \ n = 1, \\ -\left(P_1(\varphi_{\max}) + Q(\varphi_{\max})M_2\right)/\varphi_{\max}^{(m+1)/3}, \ \ n = 2; \end{cases}$$

here coefficients α_i are determined as follows: $\alpha_0 = 1$, $\alpha_3 = 2 - Q(\varphi_{\max})M_1/(3\varphi_{\max})$, $\alpha_{10} = -a_1 - Q(\varphi_{\max})M_1/(10\varphi_{\max}^{10/3})$, $\alpha_j = -Q(\varphi_{\max})M_1/(j\varphi_{\max}^{j/3})$, $j = 1, 2, 4, 5, ..., 8, 9, 11, 12, ..., m-1, m$.

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5. Numerical results

The quasifractional approximant (4.1) represents an approximate analytical expression of k, valid for all values of the spheres volume fraction $\varphi \in [0; \varphi_{\max}]$. It should be stressed that taking into account more terms of the "limiting" expansions (2.2) and (3.1) (i.e., increment m and n) leads to the growth of the accuracy of the obtained solution (4.1). Let us illustrate this dependence for the case of the SC array. We calculated k for different values of m and n. In Fig. 1 our analytical results are compared with experimental measurements of KHARADLY, JACKSON [16] and MEREDITH, TOBIAS [14]. Finally, we restrict $m = 19$ and $n = 2$ for all types of arrays, so far as it provides a satisfactory agreement with numerical data and rather simple analytical form of the solution (4.1).

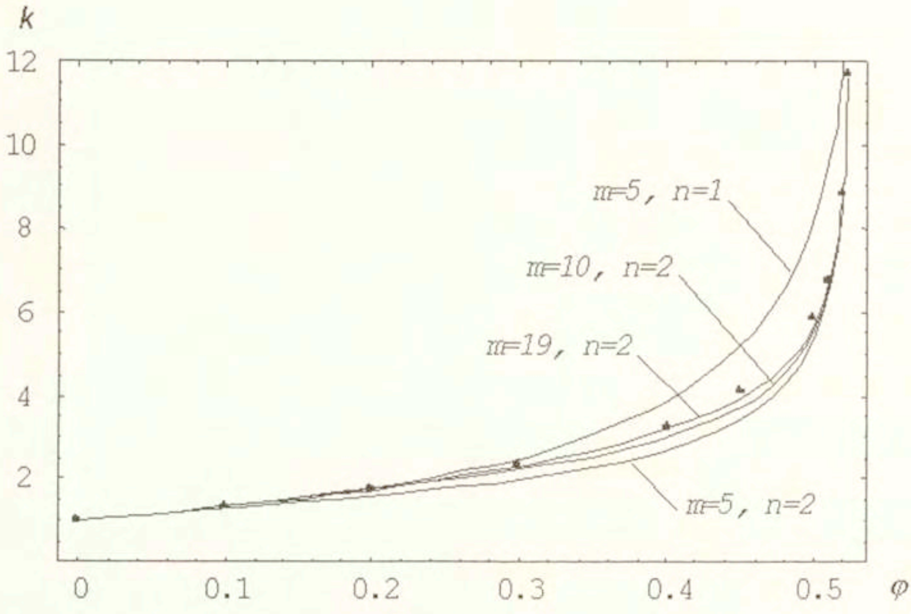

FIG. 1. Effective conductivity of the SC array. Analytical results (4.1) for different values of m, n (solid curves) are compared with experimental data [14, 16] (dots).

Numerical results for the BCC and the FCC arrays are displayed in Fig. 2 and Fig. 3 respectively. The obtained solution (4.1) is compared with experimental results of MCKENZIE *et al.* [17] for the BCC array and with numerical data [17] for the FCC array. The discrepancy between our analytical solution (4.1) and numerical results does not exceed 3.6%, 4.1% and 6.7% for, respectively, the SC, the BCC and the FCC arrays.

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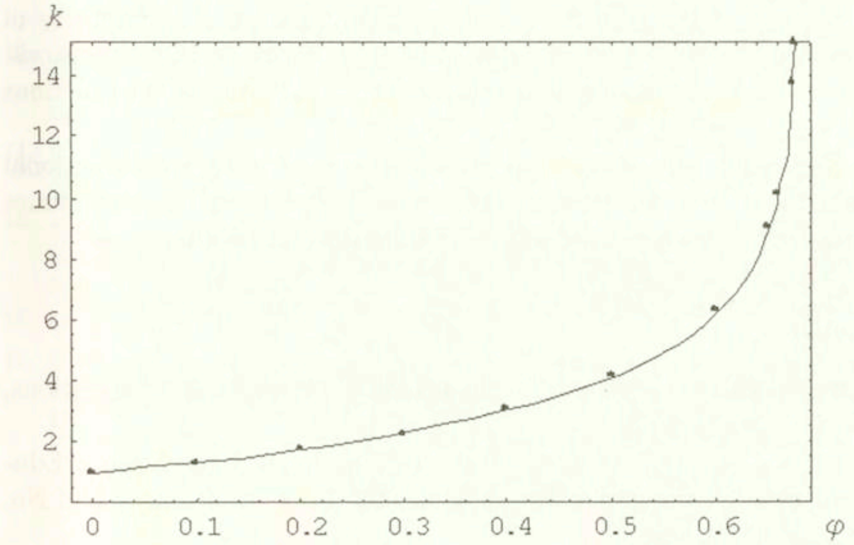

FIG. 2. The BCC array. Obtained analytical solution (4.1) (solid curve) is compared with experimental measurements [17] (dots). $m = 19$, $n = 2$.

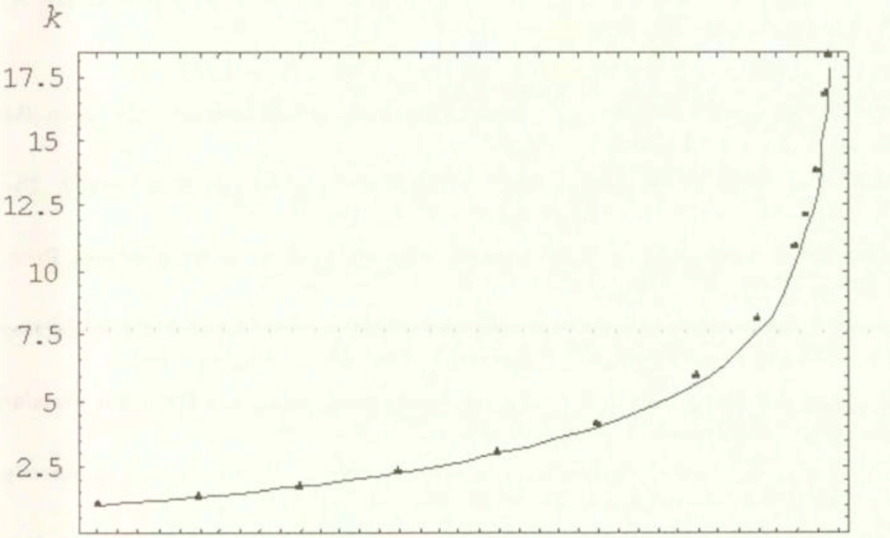

FIG. 3. The FCC array. Analytical results (4.1) (solid curve) is compared with numerical data [17] (dots). $m = 19$, $n = 2$.

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6. Concluding remarks

Main advantages of the quasifractional approximants are the simplicity of the algorithms and the possibility of using only a few terms of the expansions. Besides, it is possible to take into account the known singularities of the functions defined.

On the other hand, one of the important features of using quasifractional approximants is the control of accuracy of the realized approximation. Sometimes to this end one can use numerical methods or experimental results.

Acknowledgment

Authors are grateful to the referee for the valuable comments and suggestions, which helped us to improve the paper.

This work was supported, in part, by the International Soros Science Education Program through the grants No. SPU061002 (for I. Andrianov) and No. PSU071071 (for V. Danishevs'kyy).

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Received July 8, 1999; revised version December 30, 1999.

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