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Two-point Padé approximants to the effective heat conduction coefficient of non-uniform media

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IN [3] THE TWO-POINT PADÉ APPROXIMANTS were used to obtain the lower and upper bounds to the effective heat transfer coefficient in the composite with inclusions in the form of densely packed cylinder array. The effective heat transfer coefficient fulfils the Keller symmetry condition, however the asymptotic formula (MCPHEDRAN *et al.* [4]) used to build the approximants does not agree with this condition. By using the Keller symmetry explicitly we transform the asymptotic formula to the symmetric form and obtain better bounds than those in [3].

1. Introduction

ONE OF IMPORTANT PROBLEMS of the theory of dispersive media is the theoretical determination of the effective transport coefficient of non-uniform media on the basis of geometrical structure and physical properties of the media. In the paper we consider the effective heat conduction coefficient λ_{ef} of two-component composite with a regular square array of infinite circular cylinders immersed in an infinite matrix. The coefficients of heat conduction of inclusions and matrix are λ_d and λ_c, respectively, and the volume fraction of inclusions is φ. Our considerations are not bounded to the heat conduction theory but may be applied to other physical theories governed by the Laplace equation, such as the theory of electric conduction, dielectric constant, etc.

In most methods of investigation of the effective transport coefficient, the infinite system of algebraic equations, known as the Rayleigh equations [1], is used as the departure point. Upon truncation these equations can be solved numerically. Another method of solution is based on using the power series. However, the solution is non-analytic for $h = \lambda_d/\lambda_c$ tending to 0 or ∞ and $\varphi \to \varphi_{\max} = \pi/4$. As a consequence, both methods lose their accuracy for nearly touching cylinders, and large or small h – the power series converges very slowly in this range of parameters. In fact, while using $h-1$ or $1/(h-1)$ as the power series argument, one obtains the power series divergent in some part of the physical region. By changing the power series argument to $\alpha = (1-h)/(1+h)$ one obtains the series that converges for $|\alpha| < 1$, however the problem of slow convergence remains. Some improvement may be achieved by using the rational approximations in the form of continued fractions or Padé approximants [2]. This is due to the fact that the solution of the problem is a Stieltjes function of $h-1$ and has a set of singularities (single poles) for real $h < -1$, outside the physically meaningful region of parameters. The rational functions give better approximations to such functions. However, for $\varphi \to \varphi_{\max}$ and $h \to \infty$ an essential singularity appears and the above method fails near this singular point. For such a case MCPHEDRAN *et al.* [4] gave the asymptotic solution. There exists yet a certain gap between the solution originating from the power series at $h = 1$ (and resulting from these power series rational approximations) and the asymptotic solution. To fulfil this gap, a new approach was developed using the two-point Padé approximants. These approximants, built from the power series at $h = 1$ and the asymptotic development for $h \to \infty$ were used in [3]. There is yet a certain drawback in the method applied there. It is known [5] that the solution of our problem should fulfil the symmetry condition

$$\lambda_{ef}(1/h)\lambda_{ef}(h) = \text{const} \tag{1.1}$$

known as the Keller symmetry. Of course, the power series solution agree with the Keller symmetry, however the asymptotic solution [4], found for $h \to \infty$ (but not for $h \to 0$) fails in this respect. The same is true for the two-point Padé approximants considered in [3] and based on this asymptotic solution. In the present investigation we take into account the Keller symmetry as an additional condition. Owing to this we obtain the correct asymptotic transition not only for $h \to \infty$ but also for $h \to 0$; moreover, the approximants fulfilling the symmetry condition give better bounds to the solution than those found in [3]. The influence of analytical properties of functions, such as the Keller symmetry, on the bounds of effective properties of materials was investigated in [10] for a more general class of composites. However the type of bounds, considered in the present paper, and based on the asymptotic solution, was not particularly treated there.

2. The problem formulation and the power series solution

We consider an infinite regular system of circular cylinders in the form of a square array. Let the distance between the neighbouring cylinder axes be 1 and the cylinder radius ρ. The temperature distribution in the medium is governed by the Eq. (2.1)

$$\nabla \cdot (\lambda_c + (\lambda_d - \lambda_c)\theta_d)\nabla T = 0, \tag{2.1}$$

where θ_d is the characteristic function of cylinders. Besides the heat transfer equation one should take into account the conditions of continuity of temperature and normal component of heat flux $\mathbf{q} = (\lambda_c + (\lambda_d - \lambda_c)\theta_d)\nabla T$ on the cylinder border

$$T(\rho_-) = T(\rho_+), \qquad \mathbf{q}(\rho_-)\cdot\mathbf{n} = \mathbf{q}(\rho_+)\cdot\mathbf{n}, \tag{2.2}$$

where $\mathbf{n}$ is the unit normal vector, and the indices minus and plus correspond to the internal and external side od cylinder surface, respectively. To determine the effective heat transfer coefficient we introduce a constant external temperature gradient in the direction of the Ox-axis. The temperature distribution in the medium can be considered as the sum of the systematic $T^{(0)}$ and periodic $T^{(p)}$ components: $T = T^{(0)} + T^{(p)}$. In the problem the amplitude of $T^{(0)}$ is not important, and without any loss of generality we may put $T^{(0)} = x$. For the periodic component $T^{(p)}$ we consider the periodicity conditions on the border of elementary cell

$$\mathbf{n}\cdot\nabla T^{(p)} = 0. \tag{2.3}$$

It is convenient to seek the solution of Eq. (2.1) with the boundary conditions (2.2) and (2.3) in the functional basis derived from the Wigner potential ([2, 3, 9]). The elements of this basis fulfil the boundary conditions (2.3).

The effective heat transfer coefficient is defined as

$$\lambda_d = \left\langle (\lambda_c + (\lambda - \lambda_c)\theta_d)\,\frac{\partial T}{\partial x}\right\rangle, \tag{2.4}$$

where $\langle\ldots\rangle = S^{-1}\int\ldots dS$ means the average over the elementary cell. Expressing the temperature in the referred basis, one can define a very simple algorithm for finding the effective heat transfer coefficient as a power series of $h-1$. The algorithm was used in [3], and described in more details in [9]. Using this algorithm one can determine numerically the coefficients of the power series (2.5):

$$\frac{\lambda_{ef}}{\lambda_c} = c_0 + c_1(h-1) + c_2(h-1)^2 + \ldots. \tag{2.5}$$

3. Padé approximants and the Keller symmetry

The rational function

$$[M/M]_n = \frac{A_0 + A_1 z + \ldots + A_M z^M}{1 + B_1 z + \ldots + B_M z^M}, \tag{3.1}$$

is the two-point Padé approximant to the Stieltjes function $f(z)$ if $f(z)$ can be developed to the formal power series in 0 and infinity (convergence radius can be equal to 0) and

1. The first n coefficients of the expansion of $[M/M]_n$ to the power series of the argument $1/z$ are equal to the corresponding coefficients of the power expansion of $f(z)$ at infinity;

2. The $2M+1-n$ first coefficients of the expansion of $[M/M]_n$ to the power series of z are equal to the corresponding coefficients of the power expansion of $f(z)$ at $z=0$.

For n even or odd, the approximants give a lower or upper bound of $f(z)$, respectively. In the following we shall only consider the approximants $[M/M]_2$. They fulfil [11] the following inequality:

$$[M/M]_2 \leqslant [M+1/M+1]_2 \leqslant f(z) \tag{3.2}$$

for $z \geqslant 0$ and natural M. As a consequence of (3.2), the larger is M, the better is the bound for $f(z)$.

Using the algorithm mentioned in the previous section one can obtain λ_{ef} as a power series of $h-1$. On the other hand, the asymptotic formula given in [4] makes it possible to find the first two coefficients of the asymptotic expansion of λ_{ef} with the argument $1/h$. Using merely the two first terms of the series one may replace the argument $1/h$ in the asymptotic expansion by $1/(h-1)$. The extra terms introduced by this replacement of arguments, being of the order $O(h^{-2})$, are omitted in the given approximation. For the given approximants of both series of arguments $h-1$ and $1/(h-1)$ one can obtain the Padé approximants using for example the algorithm QD, described in [8]. Such a method, used in [3], has yet a certain deficiency. It has the same fault as the asymptotic formula in [4] – it does not agree with the Keller symmetry (1.1): it is valid for $h \to \infty$ but not for $h \to 0$. To make use of the Keller symmetry, let us introduce a new argument α instead of h

$$\alpha = \frac{1-h}{1+h} \tag{3.3}$$

and new functions β_c and β_d, instead of λ_{ef}

$$\begin{aligned} \beta_c &= \alpha\varphi\frac{1+\lambda_{ef}/\lambda_c}{1-\lambda_{ef}/\lambda_d}, \\ \beta_d &= \alpha(1-\varphi)\frac{(1+\alpha)\lambda_{ef}/\lambda_c+(1-\alpha)}{(1+\alpha)\lambda_{ef}/\lambda_c-(1-\alpha)}. \end{aligned} \tag{3.4}$$

Solving (3.4) with respect to λ_{ef}/λ_c and λ_{ef}/λ_d we obtain

$$\frac{\lambda_{ef}}{\lambda_c} = 1 - \frac{2\alpha\varphi}{1+\alpha\varphi+\beta_c},$$
(3.5)
$$\frac{\lambda_{ef}}{\lambda_d} = 1 + \frac{2\alpha(1-\varphi)}{1-\alpha(1-\varphi)+\beta_d}.$$

For β_c and β_d equal to 0 the formulae (3.5) transform to the Maxwell-Garnett formula, independent of the geometrical structure of the composite. The whole information about geometrical structure of the composite is comprised in β_c or β_d. It follows from (3.5) that the lower bound of β_c and β_d give the lower and upper bounds of λ_{ef}, respectively. Using (1.1) and (3.4) one may easily check that $\beta_i(\alpha) = \beta_i(-\alpha)$ for $i = c, d$ as a consequence of the Keller symmetry; therefore $\beta_i = \beta_i(\alpha^2)$. For $1/h \ll \sqrt{1-4\varphi/\pi} \ll 1$ the asymptotic expression of λ_{ef} from [4] simplifies to the form:

(3.6)
$$\left(\frac{\lambda_{ef}}{\lambda_c}\right)^{as} = 1 + q_0 + \frac{q_1}{h} + O(h^{-2}),$$

where

$$q_0 = \pi(\sigma - 1),$$
(3.7)
$$q_1 = -2\pi\sigma(\sigma-1)\ln\sigma,$$
$$\sigma = \frac{1}{\sqrt{1-\dfrac{4\varphi}{\pi}}}.$$

Inserting (3.6) to (3.4) one founds the asymptotic expressions for β_c and β_d:

$$\beta_c^{as} = c_{c0} + \frac{c_{c1}}{h} + O(h^{-2}),$$
(3.8)
$$\beta_d^{as} = c_{d0} + \frac{c_{d1}}{h} + O(h^{-2}),$$

where

$$c_{c0} = \frac{2\varphi}{\pi}\left(\frac{\pi}{2} + \frac{1}{\sigma-1}\right), \qquad c_{d0} = -\varphi,$$
(3.9)
$$c_{cl} = \frac{4\varphi}{\pi}\left(\frac{\sigma\ln\sigma - 1}{\sigma-1} - \frac{\pi}{2}\right), \qquad c_{d1} = 2\pi(1-\varphi)(\sigma-1).$$

The formulae (3.8) are valid for $h \to \infty$ what corresponds to $\alpha \to -1$, and do not fulfil the Keller symmetry. To transform (3.8) to the symmetric form let us note that for $h \to \infty$ the following relation $1-\alpha^2 = 4/h + O(h^{-2})$ results from (3.3). Using this relation one can transform the asymptotic formula (3.8) to the symmetrical form (3.10):

$$\tag{3.10} \begin{aligned} \beta_c^{as} &= c_{c0} + \frac{1}{4}c_{c1}(1-\alpha^2) + O\left((1-\alpha^2)^2\right), \\ \beta_d^{as} &= c_{d0} + \frac{1}{4}c_{d1}(1-\alpha^2) + O\left((1-\alpha^2)^2\right). \end{aligned}$$

Eqs. (3.10) give the first two terms of the asymptotic power series of the argument $1-\alpha^2$. They give correct asymptotic result for $h \to \infty$ and for $h \to 0$: in both cases $\alpha^2 \to 1$. For $h \to \infty$, Eqs. (3.8) and (3.10) differ by the terms $O(h^{-2})$. Upon inserting the asymptotic expressions (3.10) to (3.6) we obtain the asymptotic expression for the effective heat transfer coefficient, valid for both $h \to \infty$ and $h \to \infty$ (more exactly: for $h(1-4\varphi/\pi)^{1/2} \to \infty$ and $h(1-4\varphi/\pi)^{1/2} \to 0$ because of the limited region of applicability of the asymptotic formula (3.6)). The argument α^2 has a certain disadvantage because the functions $\beta_c(\alpha^2)$ and $\beta_d(\alpha^2)$ are not the Stieltjes functions – their poles corresponding to $h < -1$ are now located on the positive semi-axis $\alpha^2 > 1$ – while the formula (3.2) for the two-point Padé approximants is valid for the Stieltjes functions. To obtain β_c and β_d as Stieltjes functions, let us introduce a new argument t

$$\tag{3.11} t = h + \frac{1}{h} - 2 = \frac{4\alpha^2}{1-\alpha^2},$$

hence

$$\tag{3.12} \alpha^2 = 1 - \frac{1}{1-t/4}.$$

The negative values of t correspond to $h < 1$. Expressing α as a function of t and inserting it into (3.10) one obtains the following formulae for $\beta_c(\alpha^2)$ and $\beta_d(\alpha^2)$:

$$\tag{3.13} \begin{aligned} \beta_c^{as} &= c_{c0} + \frac{c_{c1}}{t} + O(t^{-2}), \\ \beta_d^{as} &= c_{d0} + \frac{c_{d1}}{t} + O(t^{-2}). \end{aligned}$$

To obtain the power expansion of β_c and β_d at $t = 0$, let us remark that

$$\tag{3.14} h - 1 = -\frac{2\alpha}{1+\alpha},$$

as it follows from (3.3). Expanding the right-hand side of (3.14) into the power series and inserting it into (2.4) one obtains λ_{ef}/λ_c as a power series of α. Upon inserting this power series into (3.4) one finds β_c and β_d as power series of α. As a consequence of the Keller symmetry, the coefficients of the odd powers of α in the series are equal to 0. Now using (3.12) and expanding α^2 into the power series of t, we obtain β_c and β_d as a power series of t

$$\beta_c = a_0 + a_1 t + a_2 t^2 + \ldots$$
(3.15)
$$\beta_d = b_0 + b_1 t + b_2 t^2 + \ldots$$

Taking as the departure point the power series (3.15) and using the algorithm FG given in [8], we obtain the two-point Padé approximants $[M/M]_2$ (see (2.1)) of β_c and β_d. Because we take into account the even number of terms of the asymptotic development (3.13) (namely two), the Padé approximants give accordingly to (3.2) lower bounds of β_c and β_d. Inserting these bounds to (3.5) we obtain upper and lower bounds for λ_{ef}, respectively.

4. Numerical results

Numerical calculations were performed for nearly touching cylinders corresponding to $\varphi \geqslant 0.785$. For smaller φ the one-point Padé approximants and the continued fractions give satisfactory results. The region of φ for which the two-point Padé approximants give good results is determined by the region in which the asymptotic formula (3.6) is valid (i.e. for $\varphi_{\max} - \varphi \ll 1$). There is yet another restraint: in the series (3.6) we consider two first terms only – it is difficult to make this formula symmetric while using more terms (and it is doubtful whether the further terms in the asymptotic expansion are correct). Therefore, although we consider the values of φ near $\varphi_{\max}$ in some sense, there is no possibility of the limit transition $\varphi \to \varphi_{\max}$ because all derivatives of λ_{ef}/λ_c with respect to h tend to infinity for $h \to \infty$ and $\varphi \to \varphi_{\max}$, and the formula based on a finite number of derivatives can not be a good approximant for φ too near to $\varphi_{\max}$.The asymptotic values of lower and upper bounds of λ_{ef} for $h \to \infty$ and $\varphi < \varphi_{\max}$ are always correct and equal one to another – it follows from the nature of the method. For φ very near to $\varphi_{\max}$, there appears however an intermediate region of large h in which the lower and upper bounds may considerably differ, and their difference tends to infinity while $\varphi \to \varphi_{\max}(\varphi_{\max} = 0.785398163...)$. On the other hand, if φ is too small the method becomes unstable. Both these constraints determine the limits within which the method is useful. The situation is analogous to that in [3] but in our case the bounds for λ_{ef} are better.

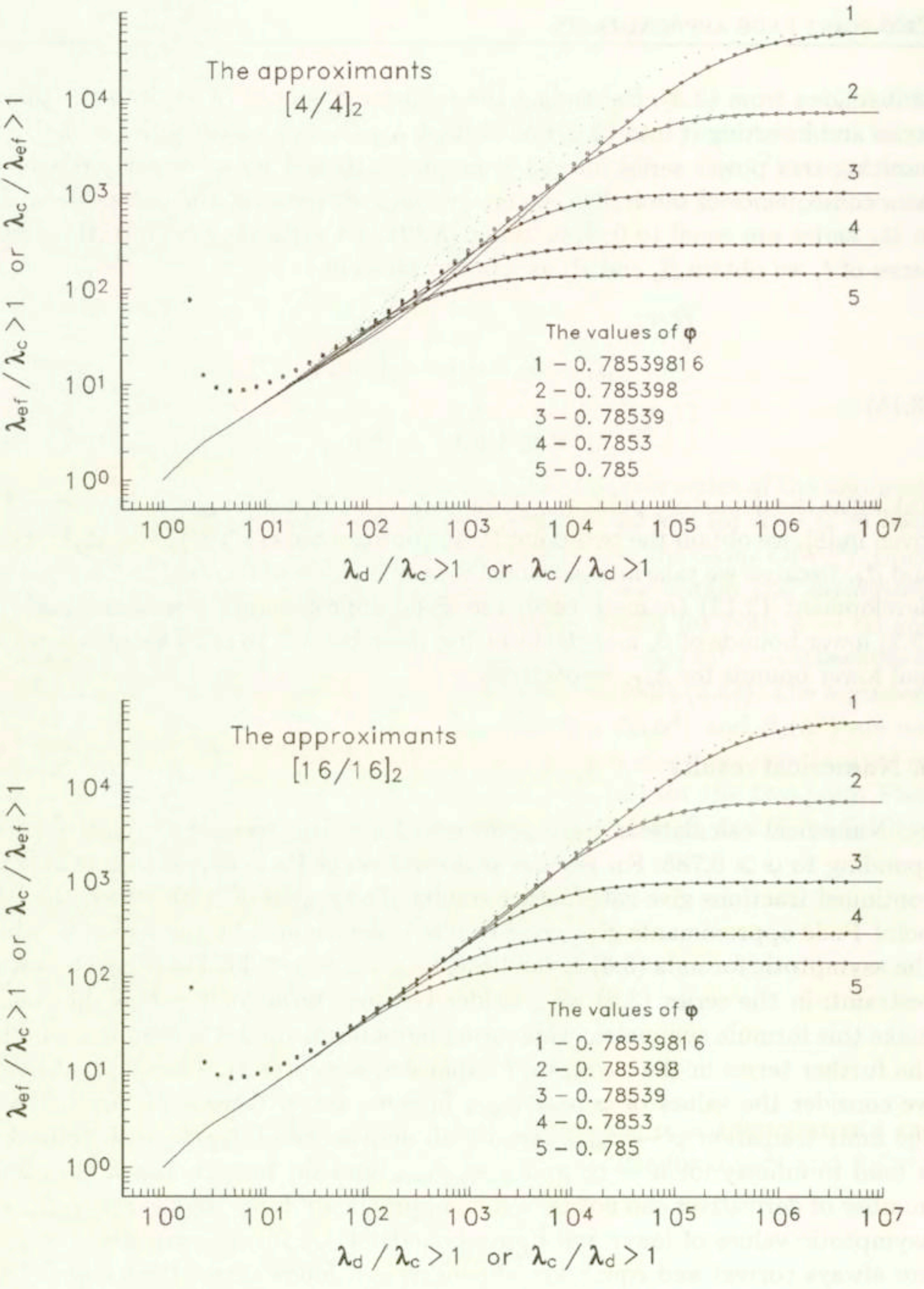

FIG. 1. The upper (dotted lines) and lower (solid lines) bounds to the effective heat transfer coefficient for the square array of nearly touching cylinders obtained from the two-point Padé approximants $[4/4]_2$ and $[16/16]_2$. For comparison, the asymptotic results (McPHEDRAN *et al.* [6]) are shown by small solid squares.

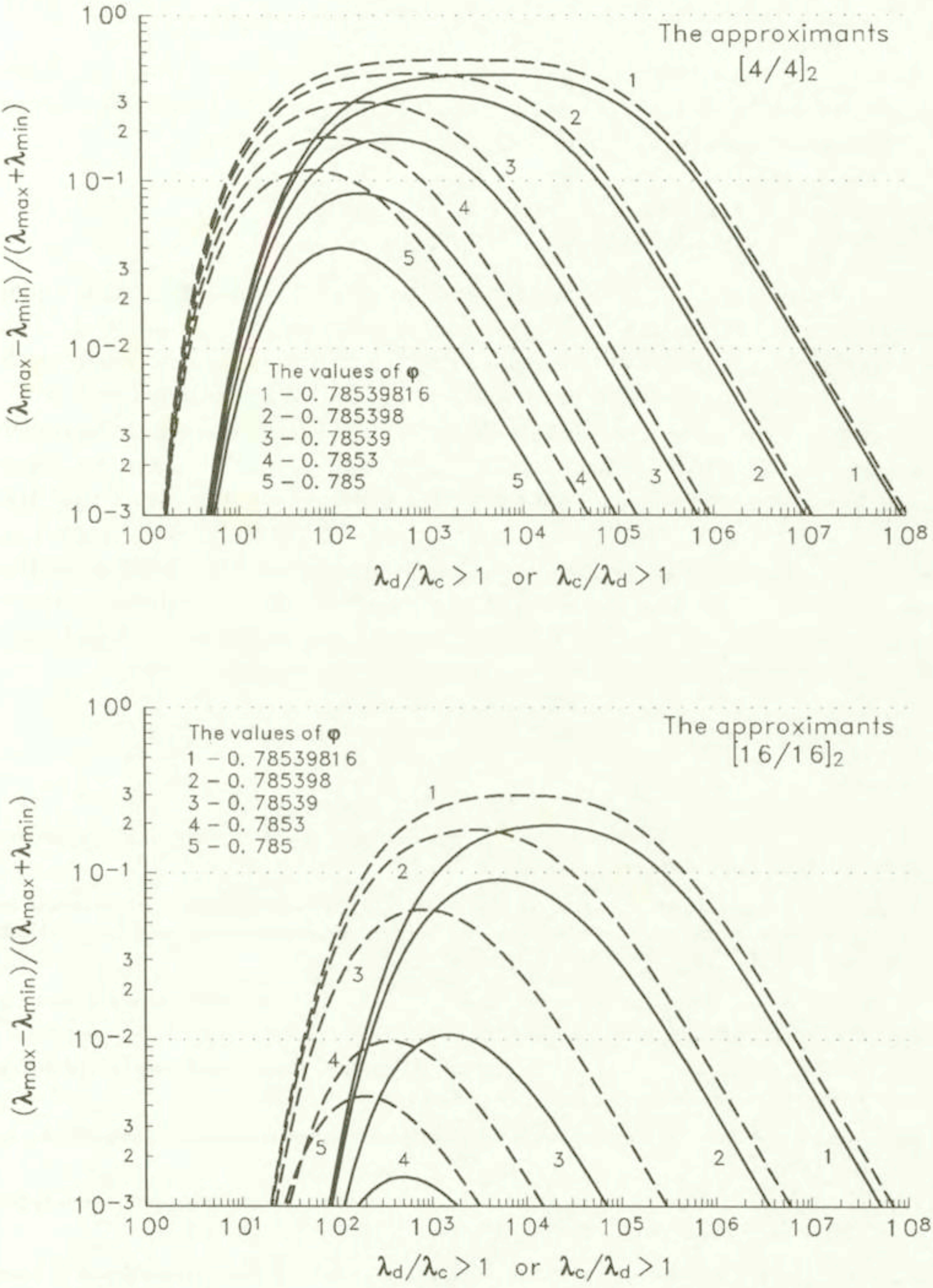

FIG. 2. The relative differences between the upper and lower bounds from Fig. 1 (solid lines) as compared with the corresponding results calculated without using the Keller symmetry [3] (dashed lines).

In the Fig. 1 the lower and upper bounds of λ_{ef} obtained from the Padé approximants $[4/4]_2$ and $[16/16]_2$ are shown. It follows from the Keller symmetry (1.1) that in the right-hand side of both equalities (4.1)

$$\frac{\lambda_{ef}}{\lambda_c} = f\left(\frac{\lambda_d}{\lambda_c}\right), \qquad \frac{\lambda_c}{\lambda_{ef}} = f\left(\frac{\lambda_c}{\lambda_d}\right) \tag{4.1}$$

appears the same function f. Because one of the ratios λ_d/λ_c and λ_c/λ_d is equal or larger than 1, the values less than 1 are not shown in the plot of f. The asymptotic values from [4] are also shown in the figure. It may be easily seen that the lower bounds are much more precise than the upper bounds (for $h > 1$).

To compare the presented results with those of [3], which disregard the Keller symmetry, the relative difference $(\lambda_{\max} - \lambda_{\min})/(\lambda_{\max} + \lambda_{\min})$ between the upper and the lower bounds is shown in the Fig. 2. It is seen from the Fig. 2 that the discrepancy between the lower and upper bounds is largest in some region of large h, and increases with φ. Of course, this discrepancy is much smaller for the $[16/16]_2$ approximants than for $[4/4]_2$. The comparison of our results with those from [3] shows that our bounds are more accurate. For the values of h not very large, the difference may be even of one order of magnitude or more.

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