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Scattering by many small particles and creating materials with a desired refraction coefficient

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Abstract: Combining an asymptotic method and computational modelling the authors propose a method for creating materials with the desired electrodynamical characteristics, in particular, with a desired refraction coefficient. The problem of wave scattering by many small particles is solved asymptotically under the assumptions $ka \ll 1$, $d \gg a$, where a is the size of the particles and d is the distance between the neighbouring particles. On the wavelength one may have many small particles. Impedance boundary conditions are assumed on the boundaries of small particles. The results of numerical simulation show good agreement with the theory. Constructive conclusions are given for creating materials with a desired refraction coefficient on the basis of the obtained numerical results. Engineering realisation of the theory is of practical interest.

Keywords: many-body wave scattering problem; desired refraction coefficient; computational modelling.

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Alexander G. Ramm is an author of more than 590 papers, 2 patents, 12 monographs, an Editor of 3 books. He is an Associate Editor

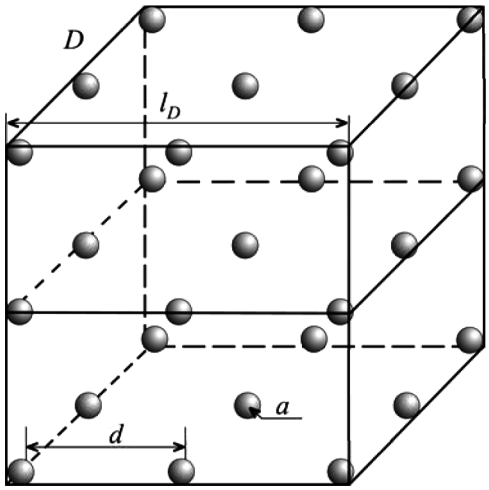
of several journals. He gave more than 140 addresses at various Conferences, visited many Universities in Europe, Asia, Australia and USA. He won Khwarizmi International Award in Mathematics, was a London Mathematical Society Speaker, distinguished HKSTAM Speaker, CNRS Research Professor, Fulbright Professor in Israel, distinguished Foreign Professor in Mexico and Egypt. His research interests include many areas of analysis, numerical analysis and mathematical physics.

1 Introduction

Theory of wave scattering by small particles of arbitrary shapes was developed by Ramm (2005a) (see also Ramm, 2005b), where analytical formulas for S-matrix for acoustic and electromagnetic wave scattering by small bodies were derived. This theory is a foundation for the proposed approach for creating materials with a desired spatial dispersion, i.e., one can create the refraction coefficient $n^2(x, \omega)$ with a desired ω-dependence, where ω is the wave frequency. In particular, one can create materials with negative refraction. Such materials are of interest in many applications, see, e.g., Seo et al. (2003), Shonbrun et al. (2005), von Rhein et al. (2007), Gregorchyk et al. (2005), and Hansen (2009).

The proposed theory allows one to calculate the S-matrix with an arbitrary accuracy and can be used in many practical problems. An asymptotically exact solution of the many-body wave scattering problem was developed in Ramm (2007) under the assumptions $ka \ll 1$, $d = O(a^{1/3})$, $M = O(1/a)$, where a is the characteristic size of the particles, $k = 2\pi/\lambda$ is the wave number, d is the distance between neighbouring particles, and M is the total number of the particles embedded in a bounded domain $D \subset R^3$. It was not assumed in Ramm (2007) that the particles were distributed uniformly in the space, or that there was any periodic structure in their distribution. In this paper, the uniform distribution of particles in D for the computational modelling is assumed (see Figure 1). An impedance boundary

Figure 1 Geometry of problem with $M = 27$ particles



condition on the boundary S_m of the mth particle D_m was assumed, $1 \leq m \leq M$. In Ramm (2008) the above assumptions were generalised as follows:

$$\zeta_m = \frac{h(x_m)}{a^\kappa}, \quad d = O(a^{(2-\kappa)/3}), \quad M = O\left(\frac{1}{a^{2-\kappa}}\right), \quad \kappa \in (0,1), \tag{1}$$

where ζ_m is the boundary impedance, $h_m = h(x_m)$, $x_m \in D_m$, and $h(x) \in C(D)$ is an arbitrary continuous in $\overline{D}$ function, $\overline{D}$ is the closure of D, $Imh \leqslant 0$.

The initial field u_0 satisfies the Helmholtz equation in R^3 and the scattered field satisfies the radiation condition. We assume in this paper that $\kappa \in (0,1)$ and the small particle D_m is a ball of radius a centred at the point $x_m \in D$, $1 \leqslant m \leqslant M$.

2 The solution of the scattering problem

The scattering problem is

$$[\nabla^2 + k^2 n_0^2(x)]u_M = 0 \quad \text{in } R^3 \setminus \bigcup_{m=1}^{M} D_m, \tag{2}$$

$$\frac{\partial u_M}{\partial N} = \zeta_m u_M \quad \text{on } S_m, \quad 1 \leqslant m \leqslant M, \tag{3}$$

where

$$u_M = u_0 + v_M, \tag{4}$$

u_0 is a solution to problem (2), (3) with $M = 0$ (i.e., in the absence of the embedded particles) and with the incident field $e^{ik\alpha\cdot x}$. The scattered field v_M satisfies the radiation condition. The refraction coefficient $n_0^2(x)$ of the material in a bounded region D is assumed for simplicity a bounded function whose set of discontinuities has zero Lebesgue measure in R^3, and $Im\, n_0^2(x) \geq 0$. In $D' := R^3 \setminus D$ we assume that $n_0^2(x) = 1$.

It was proved in Ramm (2008) that the unique solution to problem (2)–(4) exists and is of the form

$$u_M(x) = u_0(x) + \sum_{m=1}^{M} \int_{S_m} G(x,y)\sigma_m(y)dy, \tag{5}$$

where $G(x,y)$ is Green's function of the Helmholtz equation (2) in the case when $M = 0$, i.e., when there are no embedded particles, and $\sigma_m(y)$ are some unknown functions. If these functions are chosen so that the boundary conditions (3) are satisfied, then formula (5) gives the unique solution to problem (2)–(4).

Let us define the "effective field" u_e, acting on the mth particle:

$$u_e(x) := u_e(x,a) := u_e^{(m)}(x) := u_M(x) - \int_{S_m} G(x,y)\sigma_m(y)dy, \tag{6}$$

where $|x - x_m| \sim a$. The effective field is a correction to $u_M(x)$ which is essential only in the region $|x - x_m| \sim a$. If $|x - x_m| \gg a$, then $u_M(x) \sim u_e^{(m)}(x)$. The $\sim$ sign

denotes the same order as $a \to 0$. The function $\sigma_m(y)$ solves an exact integral equation (see Ramm, 2008). This equation is solved in Ramm (2008) asymptotically as $a \to 0$. These results are given in Section 3, see formulas (12)–(15) in Section 3.

Let $h(x) \in C(D)$, $Imh \leqslant 0$, be arbitrary, $\Delta_p \subset D$ be any subdomain of D, and $\mathcal{N}(\Delta_p)$ be the number of the embedded particles in Δ_p. We assume that

$$\mathcal{N}(\Delta_p) = \frac{1}{a^{2-\kappa}} \int_{\Delta_p} N(x)dx[1 + o(1)], \quad a \to 0, \tag{7}$$

where $N(x) \geqslant 0$ is a given continuous function in D. The following result was proved in Ramm (2008) (Theorem 1): there exists the limit $u(x)$ of $u_e(x)$ as $a \to 0$:

$$\lim_{a \to 0} \|u_e(x) - u(x)\|_{C(D)} = 0, \tag{8}$$

and $u(x)$ solves the following equation:

$$u(x) = u_0(x) - 4\pi \int_D G(x, y)h(y)N(y)u(y)dy. \tag{9}$$

This is the equation, derived in Ramm (2008) for the limiting effective field in the medium, created by embedding many small particles with the distribution law (7).

3 Approximate representation of the effective field

Let us derive an explicit formula for the effective field u_e. Rewrite the exact formula (5) as:

$$\begin{aligned} u_M(x) = u_0(x) &+ \sum_{m=1}^{M} G(x, x_m)Q_m \\ &+ \sum_{m=1}^{M} \int_{S_m} G(x, y) - G(x, x_m)\sigma_m(y)dy, \end{aligned} \tag{10}$$

where

$$Q_m = \int_{S_m} \sigma_m(y)dy. \tag{11}$$

Using some estimates of $G(x, y)$ (see Ramm, 2007) and the asymptotic formula for Q_m from Ramm (2008), one can rewrite the exact formula (10) as follows:

$$u_M(x) = u_0(x) + \sum_{m=1}^{M} G(x, x_m)Q_m + o(1), \quad a \to 0, \quad |x - x_m| \geqslant a. \tag{12}$$

The number $Q_m(x)$ is given by the asymptotic formula

$$Q_m = -4\pi h(x_m)u_e(x_m)a^{2-\kappa}[1 + o(1)], \quad a \to 0, \tag{13}$$

and the asymptotic formula for σ_m is (see Ramm, 2008):

$$\sigma_m = -\frac{h(x_m)u_e(x_m)}{a^\kappa}[1 + o(1)], \quad a \to 0. \tag{14}$$

The asymptotic formula for $u_e(x)$ in the region $|x - x_j| \le a$, $1 \le j \le M$, is (see Ramm, 2008):

$$u_e^{(j)}(x) = u_0(x) - 4\pi \sum_{m=1, m\neq j}^{M} G(x, x_m)h(x_m)u_e(x_m)a^{2-\kappa}[1 + o(1)]. \tag{15}$$

Equation (9) for the limiting effective field $u(x)$ is used for numerical calculations when the number M is large, e.g., $M = 10^b, b > 3$. The goal of our numerical experiments is to investigate the behaviour of the solution to equation (9) and compare it with the asymptotic formula (15) in order to establish the limits of applicability of our asymptotic approach to many-body wave scattering problem for small particles.

4 Reduction of the scattering problem to solving linear algebraic systems

The numerical calculation of the field u_e by formula (15) requires the knowledge of the numbers $u_m := u_e(x_m)$. These numbers are obtained by solving the following Linear Algebraic System (LAS):

$$u_j = u_{0j} - 4\pi \sum_{m=1, m\neq j}^{M} G(x_j, x_m)h(x_m)u_m a^{2-\kappa}, \quad j = 1, 2, \dots, M, \tag{16}$$

where $u_j = u(x_j)$, $1 \le j \le M$. This LAS is convenient for numerical calculations, because its matrix is sometimes diagonally dominant. Moreover, it follows from the results in Ramm (2009), that for sufficiently small a this LAS is uniquely solvable.

Let the union of small cubes Δ_p, centred at the points y_p, form a partition of D, and the diameter of Δ_p be $O(d^{1/2})$. For finitely many cubes Δ_p the union of these cubes may not give D. In this case we consider the smallest partition containing D and define $n_0^2(x) = 1$ in the small cubes that do not belong to D.

To find the solution to the limiting equation (9), we use the collocation method from Ramm (2009), which yields the following LAS:

$$u_j = u_{0j} - 4\pi \sum_{p=1, m\neq j}^{P} G(x_j, x_p)h(y_p)N(y_p)u_p|\Delta_p|, \quad p = 1, 2, \dots, P, \tag{17}$$

where P is the number of small cubes Δ_p, y_p is the centre of Δ_p, and $|\Delta_p|$ is volume of Δ_p.

From the computational point of view solving LAS (17) is much easier than solving LAS (16) if $P \ll M$.

We have two different LAS: one is (16), the other is (17). The first corresponds to formula (15). The second corresponds to a collocation method for solving equation (9). Solving these LAS, one can compare their solutions and evaluate the limits of applicability of the asymptotic approach from Ramm (2008) to solving many-body wave scattering problem in the case of small particles.

5 Numerical experiments

The numerical approach to solving the wave scattering problem for small particles was developed in Andriychuk and Ramm (2009). There some numerical results were given. These results demonstrated the applicability of the asymptotic approach to solving many-body wave scattering problem by the method described in Sections 3 and 4.

From the practical point of view, the following numerical experiments are of interest and of importance:

a For not very large M, say, $M = 2$, 5, 10, 25, 50, one wants to find a and d, for which the asymptotic formula (12) (without the remainder $o(1)$) is no longer applicable

b One wants to find the relative accuracy of the solutions to the limiting equation (9) and of the LAS (17)

c For large M, say, $M = 10^5$, $M = 10^6$, one wants to find the relative accuracy of the solutions to the limiting equation (9) and of the solutions to LAS (16)

d One wants to find the relative accuracy of the solutions to LAS (16) and (17)

e Using Ramm's method for creating materials with a desired refraction coefficient, one wants to find out for some given refraction coefficients $n^2(x)$ and $n_0^2(x)$, what the smallest M (or, equivalently, largest a) is for which the corresponding $n^2_{M(x)}$ differs from the desired $n^2(x)$ by not more than, say, 5%–10%. Here $n^2_{M(x)}$ is the value of the refraction coefficient of the material obtained by embedding M small particles into D accoring to the recipe described below.

We take $k = 1$, $\kappa = 0.9$, and $N(x) = \text{const}$ for the numerical calculations. For $k = 1$, and a and d, used in the numerical experiments, one can have many small particles on the wavelength. Therefore, the multiple scattering effects are not negligible.

5.1 Applicability of asymptotic formulas for small number of particles

We consider the solution to LAS (17) with 20 collocation points along each coordinate axis as the benchmark solution. The total number P of the collocation points is $P = 8000$. The applicability of the asymptotic formulas is checked by solving LAS (16) for small number M of particles and determining the problem parameters for which the solutions to these LAS are close. A standard interpolation procedure is used in order to obtain the values of the solution to (17) at the points corresponding to the position of the particles. In this case the number P of the collocation points exceeds the number M of particles. In Figure 2, the relative error of real (solid line) and imaginary (dashed line) parts, as well as the modulus (dot-dashed line) of the solution to (16) are shown for the case $M = 4$; the distance between particles is $d = a^{(2-\kappa)/3}C$, where C is an additional parameter of optimisation (in our case $C = 5$, that yields the smallest error of deviation of etalon and asymptotic field components), $N(x) = 5$. The minimal relative error of the solution to (16) does not exceed 0.05% and is reached when $a \in (0.02, 0.03)$. The value of the function $N(x)$ influences (to a considerable degree) the quality of

approximation. The relative error for $N(x) = 40$ with the same other parameters is shown in Figure 3. The error is smallest at $a = 0.01$, and it grows when a increases. The minimal error that we were able to obtain for this case is about 0.01% .

Figure 2 Relative error of solution to (16) vs. size a of particle, $N(x) = 5$

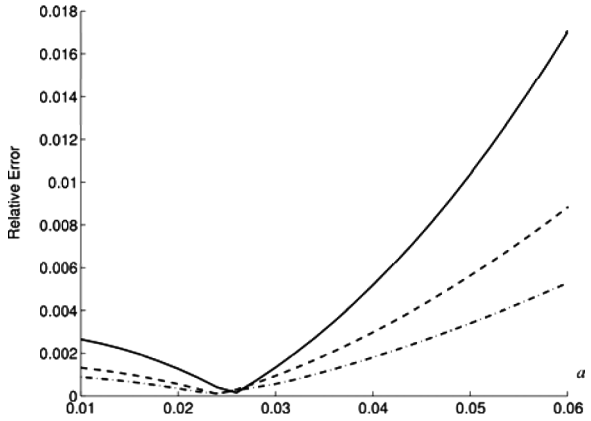
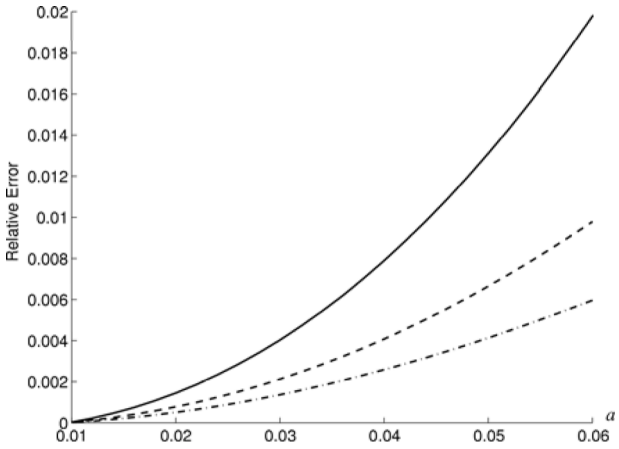


Figure 3 Relative error of solution to (16) vs. size a of particle, $N(x) = 40$



The dependence of the error on the distance d between particles for a fixed a was investigated as well. In Figure 4, the relative error vs. parameter d is shown. The number of particles $M = 4$, the radius of particles $a = 0.01$. The minimal error was obtained when $C = 14$. This error was 0.005% for the real part, 0.0025% for the imaginary part, and 0.002% for the modulus of the solution. In Figure 4 and in Figures 5–11, the solid, dashed, and dot-dashed lines correspond to error of real, imaginary parts, and modulus of solution, respectively.

The error grows significantly when d deviates from the optimal value, i.e., the value of d for which the error of the calculated solution to LAS (16) is minimal. Similar results are obtained for the case $a = 0.02$ (see Figure 5). For example, at $M = 2$ the optimal value of d is 0.038 for $a = 0.01$, and it is 0.053 for $a = 0.02$.

The error is even more sensitive to changes of the distance d in this case. The minimal value of the error is obtained when $C = 8$. The error was 0.0078% for the real part, 0.0071% for the imaginary part, and 0.002% for the modulus of the solution.

Figure 4 Relative error of solution vs. distance d between particles, $a = 0.01$

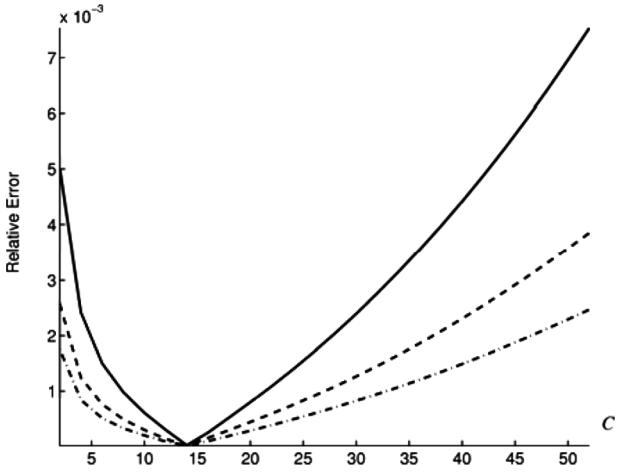
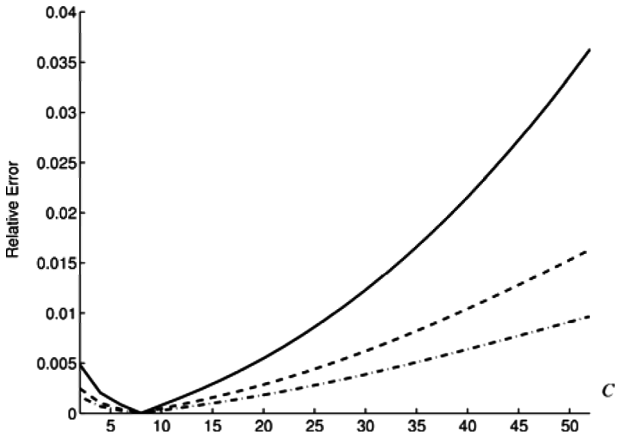


Figure 5 Relative error of solution vs. distance d between particles, $a = 0.02$



The numerical results show that the accuracy of the approximation of the solutions to LAS (16) and (17) depends on a significantly, and it improves when a decreases. For example, the minimal error, obtained at $a = 0.04$, is equal to 0.018%.

The optimal values of d are given in Tables 1 and 2 for small and not so small M respectively. The numerical results show that the distribution of particles in the medium does not influence significantly the optimal values of d. By optimal values of d we mean the values at which the error of the solution to LAS (16) is minimal when the values of the other parameters are fixed. For example, the optimal values of d for $M = 8$ at the two types of the distribution of particles: $(2 \times 2 \times 2)$ and $(4 \times 2 \times 1)$

differ by not more than 0.5%. The numerical results demonstrate that to decrease the relative error of solution to system (16), it is necessary to make a smaller if the value of d is fixed. One can see that the quality of approximation improves as $a \to 0$, but the condition $d \gg a$ is not valid for small number M of particles: the values of the distance d is of the order $O(a)$.

Table 1 Optimal values of d for small M

	M value			
	$M = 2$	$M = 4$	$M = 6$	$M = 8$
$a = 0.01$	0.038	0.025	0.026	0.027
$a = 0.02$	0.053	0.023	0.027	0.054

Table 2 Optimal values of d for medium M

	M value			
	$M = 10$	$M = 20$	$M = 30$	$M = 40$
$a = 0.01$	0.011	0.0105	0.007	0.006
$a = 0.02$	0.016	0.018	0.020	0.023

5.2 Accuracy of the solution to the limiting equation

The numerical procedure for checking the accuracy of the solution to equation (9) uses the calculations with various values of the parameters k, a, l_D, and $h(x)$. The absolute and relative errors were calculated by increasing the number of collocation points. The dependence of the accuracy on the parameter ρ, where $\rho = \sqrt[3]{P}$, P is the total number of small subdomains in D, is shown in Figures 6 and 7 for $k = 1.0$, $l_D = 0.5$, $a = 0.01$ at the different values of $h(x)$. The solution corresponding to $\rho = 20$ is considered as 'exact' solution (the number P for this case is equal to 8000).

Figure 6 Relative error vs. the ρ parameter, $h(x) = k^2(1 - 7i)/(40\pi)$

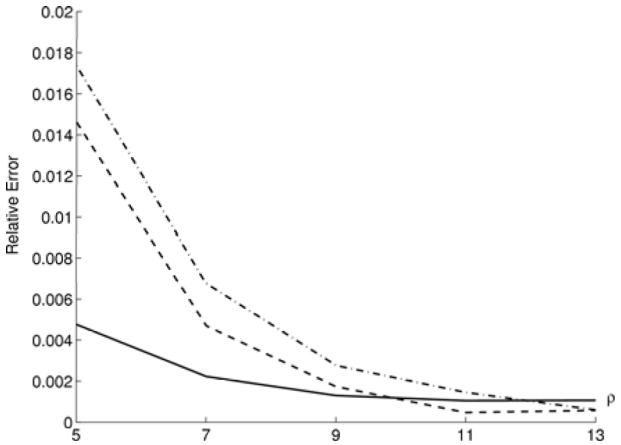
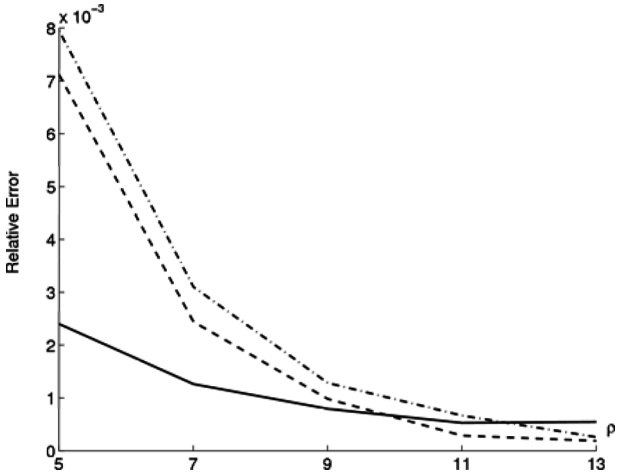


Figure 7 Relative error vs. the ρ parameter, $h(x) = k^2(1-3i)/(40\pi)$



The error of the solution to equation (9) is equal to 1.1% and 0.2% for real and imaginary part, respectively, at $\rho = 5$ (125 collocation points), it decreases to values of 0.7% and 0.05% if $\rho = 6$ (216 collocation points), and it decreases to values 0.29% and 0.02% if $\rho = 8$ (512 collocation points), $h(x) = k^2(1-3i)/(40\pi)$. The relative error smaller than 0.01% for the real part of solution is obtained at $\rho = 12$, this error tends to zero when ρ increases. This error depends on the function $h(x)$ as well, it diminishes when the imaginary part of $h(x)$ decreases. The error for the real and imaginary parts of the solution at $\rho = 19$ does not exceed 0.01%.

The numerical calculations show that the error depends much on the value of k. In Figures 8 and 9 the results are shown for $k = 2.0$ and $k = 0.6$ respectively ($h(x) = k^2(1-3i)/(40\pi)$). It is seen that the error is nearly 10 times larger at $k = 2.0$. The maximal error (at $\rho = 5$) for $k = 0.6$ is less than 30% of the error for $k = 1.0$. This error tends to zero even faster for smaller k.

Figure 8 Relative error vs. the ρ parameter, $k = 2.0$

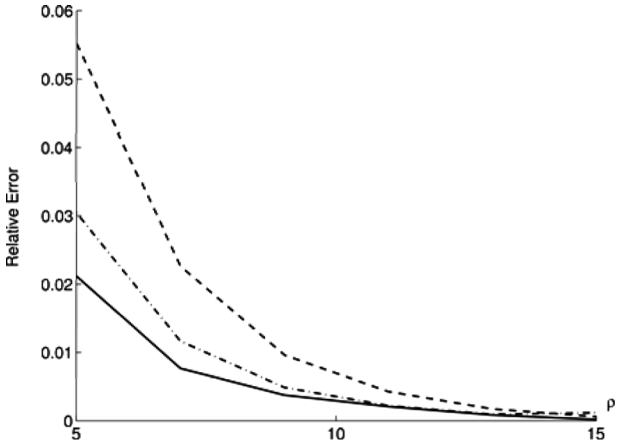
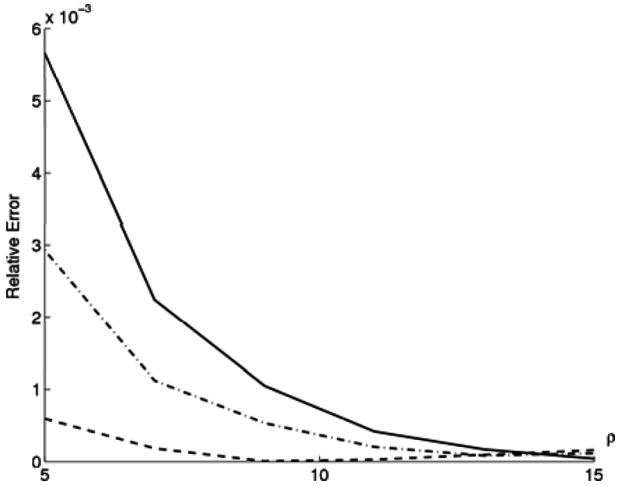


Figure 9 Relative error vs. the ρ parameter, $k = 0.6$



5.3 *Accuracy of the solution to the limiting equation (9) and of the asymptotic LAS (16)*

As before, we consider as the 'exact' solution to (9) the approximate solution to LAS (17) with $\rho = 20$. The maximal relative error for such ρ does not exceed 0.01% in the range of problem parameters we have considered ($k = 0.5 \div 1.0$, $l_D = 0.5 \div 1.0$, $N(x) \geq 4.0$). The numerical calculations are carried out for various sizes of the domain D and various function $N(x)$. The results for small values of M are presented in Table 3 for $k = 1$, $N(x) = 40$, and $l_D = 1.0$. The second line contains the values of a_{est}, the estimated value of a, calculated by formula (7), with the number $\mathcal{N}(\Delta_p)$ replacing the number M. In this case the radius of a particle is calculated as

$$a_{\text{est}} = \left(M / \int_{\Delta_p} N(x)dx \right)^{1/(2-\kappa)}. \tag{18}$$

The values of a_{opt} in the third line correspond to optimal values of a which yield minimal relative error of the modulus of the solutions to equation (9) and LAS (16). The fourth line contains the values of the distance d between particles. The maximal value of the error is obtained when $\mu = 7$, $\mu = \sqrt[3]{M}$ and it decreases slowly when μ increases. The calculation results for large number of μ with the same set of input parameters are shown in Table 4. The minimal error of the solutions is obtained at $\mu = 60$ (total number of particles $M = 2.16 \times 10^5$.

Table 3 Optimal parameters of D for small μ, $N(x) = 40.0$

μ	*7*	*9*	*11*	*13*	*15*
a_{est}	0.1418	0.0714	0.0413	0.0262	0.0177
a_{opt}	0.1061	0.0612	0.0382	0.0261	0.0172
d	0.1333	0.1105	0.0924	0.0790	0.0688
Rel. error	2.53%	0.46%	0.45%	1.12%	0.81%

Table 4 Optimal parameters of D for big μ, $N(x) = 40.0$

μ	*20*	*30*	*40*	*50*	*60*
a_{est}	0.0081	0.0027	0.0012	6.65×10^{-4}	4.04×10^{-4}
a_{opt}	0.0077	0.0025	0.0011	6.61×10^{-4}	4.04×10^{-4}
d	0.0526	0.0345	0.0256	0.0204	0.0169
Rel. error	0.59%	0.35%	0.36%	0.27%	0.19%

Tables 5 and 6 contain similar results for $N(x) = 4.0$, other parameters being the same. It is seen that the relative error of the solution decreases when number of particles M increases. This error can be decreased slightly (on 0.02%–0.01%) by small change of the values a and l_D as well. The relative error of the solution to LAS (16) tends to the relative error of the solution to LAS (17) when the parameter μ becomes greater than 80 ($M = 5.12 \cdot 10^5$). The relative error of the solution to LAS (17) is calculated by taking the norm of the difference of the solutions to (17) with P and $2P$ points, and dividing it by the norm of the solution to (17) calculated for $2P$ points. The relative error of the solution to LAS (16) is calculated by taking the norm of the difference between the solution to (16), calculated by an interpolation formula at the points y_p from (17), and the solution of (17), and dividing the norm of this difference by the norm of the solution to (17).

Table 5 Optimal parameters of D for small μ, $N(x) = 4.0$

μ	*7*	*9*	*11*	*13*	*15*
a_{est}	0.0175	0.0088	0.0051	0.0032	0.0022
a_{opt}	0.0179	0.0090	0.0052	0.0033	0.0022
d	0.1607	0.1228	0.0990	0.0828	0.0711
Rel. error	1.48%	1.14%	1.06%	1.05%	0.91%

Table 6 Optimal parameters of D for big μ, $N(x) = 4.0$

μ	*20*	*30*	*40*	*50*	*60*
a_{est}	9.97×10^{-4}	3.30×10^{-4}	1.51×10^{-4}	8.20×10^{-5}	4.98×10^{-5}
a_{opt}	1.02×10^{-3}	3.32×10^{-4}	1.50×10^{-4}	8.21×10^{-5}	4.99×10^{-5}
d	0.0542	0.0361	0.0265	0.0209	0.0172
Rel. error	0.21%	0.12%	0.11%	0.07%	0.03%

5.4 Investigation of the relative difference between the solution to (16) and (17)

A comparison of the solutions to LAS (16) and (17) is done for various values of a, and various values of the number ρ and μ. The relative error of the solution decreases when ρ grows and μ remains the same. For example, when ρ increases by 50% , the relative error decreases by 12% (for $\rho = 8$ and $\rho = 12$, $\mu = 15$).

The difference between the real parts, imaginary parts, and moduli of the solutions to LAS (16) and (17) are shown in Figures 10 and 11 for $\rho = 7$, $\mu = 15$.

The real part of this difference does not exceed 4% when $a = 0.01$, it is less than 3.5% at $a = 0.008$, less than 2% at $a = 0.005$; $d = 8a$, $N(x) = 20$. This difference is less than 0.08% when $\rho = 11$, $a = 0.001$, $N = 30$, and $d = 15a$ (μ remains the same). Numerical calculations for wider range of the distance d demonstrate that there is an optimal value of d, starting from which the deviation of solutions increases again. These optimal values of d are shown in Table 7 for various $N(x)$. The calculations show that the optimal distance between particles increases when the number of particles grows. For small number of particles (see Tables 1 and 2) the optimal distance is the value of the order a. For the number of particles $M = 15^3$, i.e., $\mu = 15$, this distance is about $10a$.

Figure 10 Deviation of component field vs. the distance d between particles, $N(x) = 10$

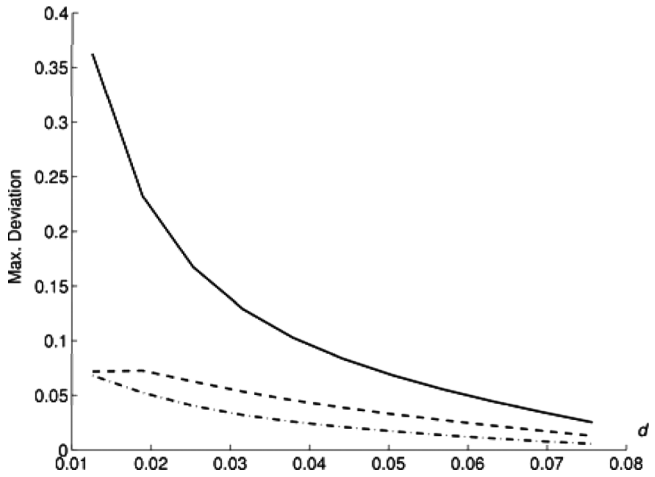
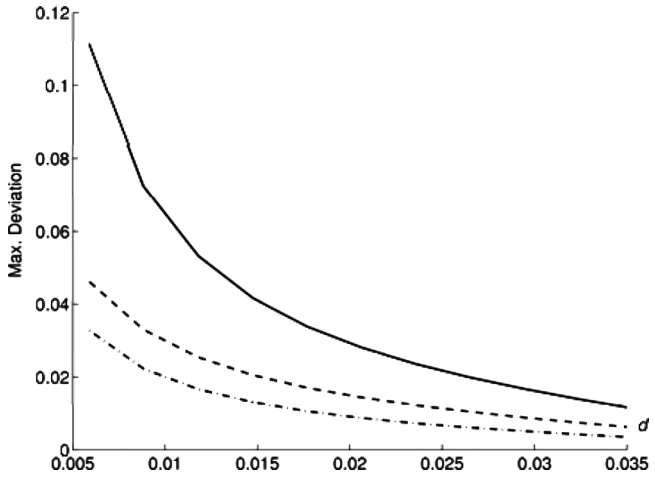


Figure 11 Deviation of component field vs. the distance d between particles, $N(x) = 30$



The values of maximal and minimal errors of the solutions for the optimal values of distance d are shown in Table 8.

Table 7 Optimal values of d for various $N(x)$

	$N(x)$ *value*				
	$N(x) = 10$	$N(x) = 20$	$N(x) = 30$	$N(x) = 40$	$N(x) = 50$
$a = 0.005$	0.07065	0.04724	0.04716	0.04709	0.04122
$a = 0.001$	0.08835	0.07578	0.06331	0.06317	0.05056

Table 8 Relative error of solution in % (max/min) for optimal d

	$N(x)$ *value*				
	$N(x) = 10$	$N(x) = 20$	$N(x) = 30$	$N(x) = 40$	$N(x) = 50$
$a = 0.005$	0.77/0.12	5.25/0.56	0.52/0.1	0.97/0.12	0.32/0.05
$a = 0.001$	2.47/0.26	1.7/0.3	0.5/0.1	2.7/0.37	1.5/0.2

One can conclude from the numerical results that optimal values of d decrease slowly when the function $N(x)$ increases. This decreasing is more pronounced for smaller a. The relative error of the solution to (16) also smaller for smaller a.

5.5 Evaluation of difference between the desired and obtained refraction coefficients

The recipe for creating the media with a desired refraction coefficient $n^2(x)$ was proposed in Ramm (2008). It is important from the computational point of view to see how the refraction coefficient $n_M^2(x)$, created by this procedure, differs from the one, obtained theoretically. First, we describe the recipe from Ramm (2008) for creating the desired refraction coefficient $n^2(x)$. By $n_0^2(x)$ we denote the refraction coefficient of the given material.

The recipe consists of three steps.

Step 1: *Given* $n_0^2(x)$ *and* $n^2(x)$, *calculate*

$$\bar{p}(x) = k^2[n_0^2(x) - n^2(x)] = \bar{p}_1(x) + i\bar{p}_2(x). \tag{19}$$

Step 1 is trivial from the computational and theoretical viewpoints.

Using the relation

$$\bar{p}(x) = 4\pi h(x)N(x) \tag{20}$$

from Ramm (2008) and equation (19), one gets the equation for finding $h(x) = h_1(x) + ih_2(x)$, namely:

$$4\pi[h_1(x) + ih_2(x)]N(x) = \bar{p}_1(x) + i\bar{p}_2(x). \tag{21}$$

Therefore,

$$N(x)h_1(x) = \frac{\bar{p}_1(x)}{4\pi}, \quad N(x)h_2(x) = \frac{\bar{p}_2(x)}{4\pi}. \tag{22}$$

Step 2: *Given* $\bar{p}_1(x)$ *and* $\bar{p}_2(x)$, *find* $\{h_1(x), h_2(x), N(x)\}$.

The system (22) of two equations for the three unknown functions $h_1(x)$, $h_2(x) \leq 0$, and $N(x) \geq 0$, has infinitely many solutions $\{h_1(x), h_2(x), N(x)\}$.

If, for example, one takes $N(x)$ to be an arbitrary positive constant, then h_1 and h_2 are uniquely determined by (22). The condition $Im\, n^2(x) > 0$ implies $Im\, \bar{p} = \bar{p}_2 < 0$, which agrees with the condition $h_2 < 0$ if $N(x) \geq 0$. One takes $N(x) = h_1(x) = h_2(x) = 0$ at the points at which $\bar{p}_1(x) = \bar{p}_2(x) = 0$.

One can choose, for example, N to be a positive constant:

$$N(x) = N = \text{const}, \tag{23}$$

$$h_1(x) = \frac{\bar{p}_1(x)}{4\pi N}, \quad h_2(x) = \frac{\bar{p}_2(x)}{4\pi N}. \tag{24}$$

Calculation of the values $N(x)$, $h_1(x)$, $h_2(x)$ by formulas (24)–(25) completes *Step 2* our procedure.

Step 2 is easy from computational and theoretical viewpoints.

Step 3: This step is clear from the theoretical point of view, but it requires solving two basic technological problems. First, one has to embed many (M) small particles into D at the approximately prescribed positions according to formula (7). Secondly, the small particles have to be prepared so that they have prescribed boundary impedances $\zeta_m = h(x_m)a^{-\kappa}$, see formula (1).

Consider a partition of D into union of small cubes Δ_p, which have no common interior points, and which are centred at the points $y^{(p)}$, and embed in each cube Δ_p the number

$$\mathcal{N}(\Delta_p) = \left[\frac{1}{a^{2-\kappa}} \int_{\Delta_p} N(x)dx \right] \tag{25}$$

of small balls D_m of radius a, centred at the points x_m, where $[b]$ stands for the integer nearest to $b > 0$, $\kappa \in (0, 1)$. Let us put these balls at the distance $O(a^{\frac{2-\kappa}{3}})$, and prepare the boundary impedance of these balls equal to $\frac{h(x_m)}{a^\kappa}$, where $h(x)$ is the function, calculated in Step 2 of our recipe.

It is proved in Ramm (2008) that the resulting material, obtained by embedding small particles into D by the above recipe, will have the desired refraction coefficient $n^2(x)$ with an error that tends to zero as $a \to 0$.

Let us emphasise again that Step 3 of our procedure requires solving the following technological problems:

(i) *How does one prepare small balls of radius a with the prescribed boundary impedance?*

(ii) *How does one embed these small balls in a given domain D, filled with the known material according to the requirements formulated in Step 3?*

Our numerical results allow one to understand better the role of various parameters, such as a, M, d, ζ, in an implementation of our recipe.

We give the numerical results for $N(x) = \text{const}$. For simplicity, we assume that the domain D is a union of small cubes subdomains Δ_p ($D = \bigcup_{p=1}^{P} \Delta_p$). This assumption is not a restriction in practical applications.

Let the functions $n_0^2(x)$ and $n^2(x)$ be given. One can calculate the values h_1 and h_2 in (24) and determine the number $\mathcal{N}(\Delta_p)$ of the particles embedded into D. The value of the boundary impedance $\frac{h(x_m)}{a^\kappa}$ is easy to calculate. Formula (25) gives the total number of the embedded particles. We consider a simple distribution of small particles. Let us embed the particles at the nodes of a uniform grid at the distances $d = O(a^{\frac{2-\kappa}{3}})$.

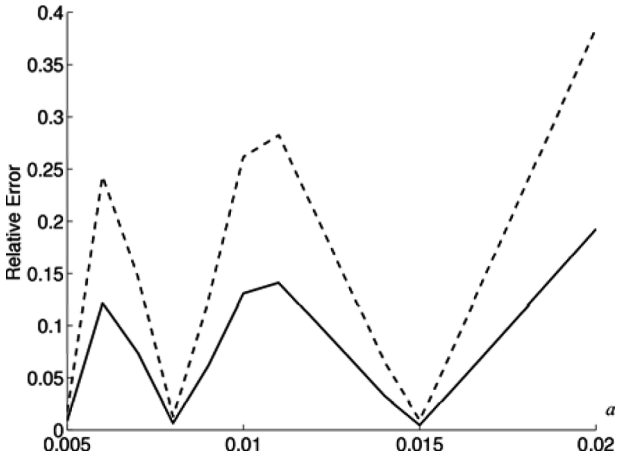
The numerical calculations are carried out for the case $D = \bigcup_{p=1}^{P} \Delta_p, P = 8000$, D is cube with side $l_D = 0.5$, the particles are embedded uniformly in D. For this P the relative error in the solution to LAS (16) and (17) does not exceed 0.1%. Let the domain D be placed in the free space, namely $n_0^2(x) = 1$, and the desired refraction coefficient be $n^2(x) = 2 + 0.01i$. One can calculate the value of $\mathcal{N}(\Delta_p)$ by formula (25). On the other hand, one can chose the number μ, such that $M = \mu^3$ is closest to $\mathcal{N}(\Delta_p)$. The corresponding $n^2(x)$ for this M, calculated by the formulas

$$\tilde{n}_1^2(x) = -\frac{4\pi M h_1}{k^2} + n_0^2, \quad \tilde{n}_2^2(x) = -\frac{4\pi M h_1}{k^2}, \tag{26}$$

differs from the desired coefficients $n_1^2(x)$ and $n_2^2(x)$. To obtain minimal error, we chose two numbers μ_1 and μ_2 such that $M_1 < \mathcal{N}(\Delta_p) < M_2$, where $M_1 = \mu_1^3$ and $M_2 = \mu_2^3$. Hence, having the number $\mathcal{N}(\Delta_p)$ for the fixed a, we can estimate the numbers M_1 and M_2, and calculate the approximate values of $n_1^2(x)$ and $n_2^2(x)$ by formula (26).

In Figure 12, the minimal relative error of the calculated value $\tilde{n}^2(x)$ depending on the radius a of particle is shown for the case $N(x) = 5$ (the solid line corresponds to the real part of the error, and the dashed line corresponds to the imaginary part of the error in Figures 12–14).

Figure 12 Minimal relative error for calculated refraction coefficient $\tilde{n}^2(x), N(x) = 5$



These results show that the error depends significantly on the relation between the numbers M_1, M_2, and $\mathcal{N}(\Delta_p)$. The error is smallest when one of the values M_1 and M_2 is sufficiently close to $\mathcal{N}(\Delta_p)$. The error has periodic nature with respect to value of a (it is clear from behaviour of the function $\mathcal{N}(\Delta_p)$ and values M_1 and

Figure 13 Minimal relative error for calculated refraction coefficient $\tilde{n}^2(x), N(x) = 20$

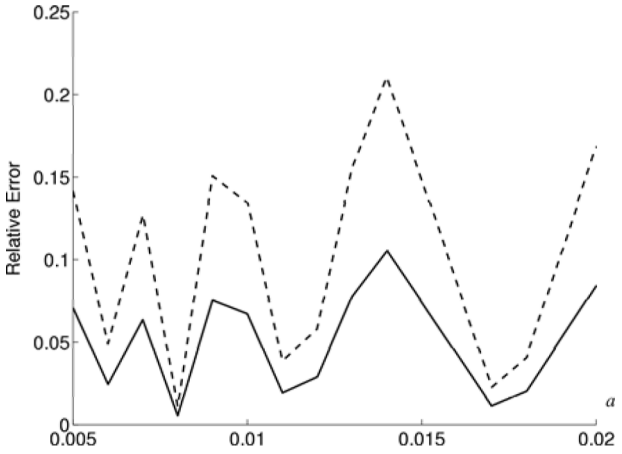
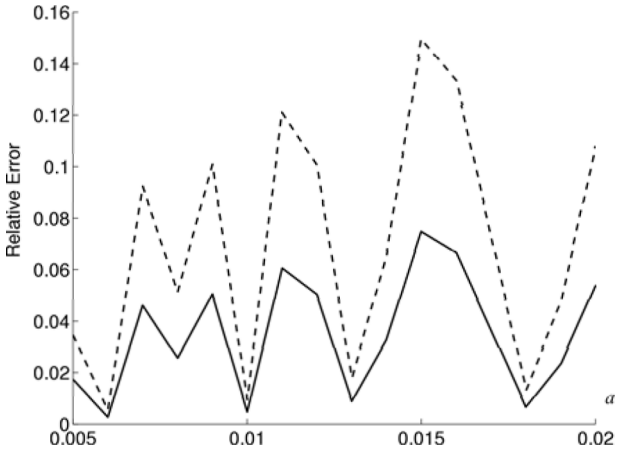


Figure 14 Minimal relative error for calculated refraction coefficient $\tilde{n}^2(x), N(x) = 50$



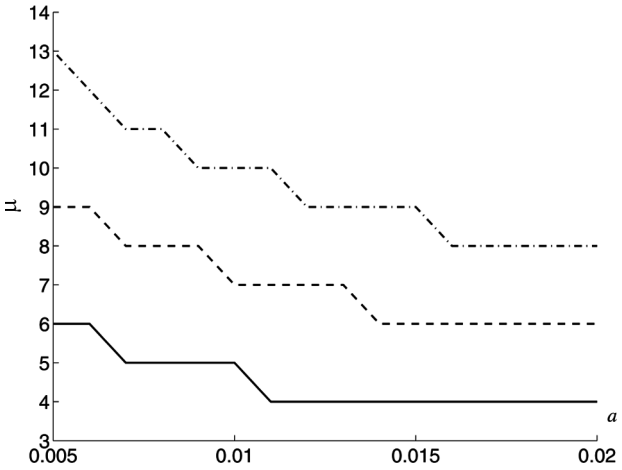
M_2). The average error on a period increases as a grows. Similar results are shown in Figures 13 and 14 for $N = 20$ and $N = 50$ respectively.

The minimal error is reached at $a = 0.015$ and equals to 0.49% , it is equal to 0.51% at $a = 0.008$, and it is equal to 0.26% at $a = 0.006$ for $N(x) = 5, 20, 50$ respectively.

Uniform (equidistant) embedding small particles into D is simple from the practical point of view. The results in Figures 12–14 allow one to estimate the number M of particles needed for obtaining the refraction coefficient close to a desired one in a given domain D. The results for $l_D = 0.5$ are shown in Figure 15. The value $\mu = \sqrt[3]{M}$ is marked on the y axes here. Solid, dashed, and dot-dashed line correspond to $N(x) = 5, 20, 50$, respectively.

One can see from Figure 15 that the number of particles decreases if radius a increases. The value $d = O(a^{(2-\kappa)/3})$ gives the distance d between the embedded particles. For example, for $N(x) = 5$, $a = 0.01$ d is of the order 0.1359, the calculated

Figure 15 Optimal value of μ vs. the radius a for various $N(x)$



d is equal to 0.12 and to 0.16 for $\mu = 5$ and $\mu = 4$, respectively. The calculations show that the difference between the both values of d is proportional to the relative error for the refraction coefficients.

By the formula $d = O(a^{(2-\kappa)/3})$, the value of d does not depend on the diameter of D. This value can be used as an additional optimisation parameter in the procedure of the choice between two neighbouring μ in Tables 9 and 10. On the other hand, one can estimate the number of the particles embedded into D using formula (24). Given $\mathcal{N}(\Delta_p)$, one can calculate the corresponding number M of particles if the particles distribution is uniform. The distance between particles is also easy to calculate if l_D is given. The optimal values of $\mu, \mu = \sqrt[3]{M}$ are shown in Tables 9 and 10 for $l_D = 0.5$ and $l_D = 1.0$ respectively.

Table 9 Optimal values of μ for $l_D = 0.5$

a	$\mathcal{N}(\Delta_p)$	*Optimal* μ
0.02	92.42	$4 \leq \mu \leq 5$
0.01	198.11	$4 \leq \mu \leq 5$
0.008	253.22	$6 \leq \mu \leq 7$
0.005	424.66	$7 \leq \mu \leq 8$
0.001	2494.1	$13 \leq \mu \leq 14$

Table 10 Optimal values of μ for $l_D = 1.0$

a	$\mathcal{N}(\Delta_p)$	*Optimal* μ
0.02	739.38	$9 \leq \mu \leq 10$
0.01	1584.9	$11 \leq \mu \leq 12$
0.008	2025.8	$12 \leq \mu \leq 13$
0.005	3397.3	$15 \leq \mu \leq 16$
0.001	19953	$27 \leq \mu \leq 28$

The numerical calculations show that the relative error of $\tilde{n}^2(x)$ for respective μ can be decreased when the estimation of d is taken into account. Namely, one should choose μ from Tables 9 or 10 that gives value of d close to $(a^{(2-\kappa)/3})$.

6 Conclusions

The numerical results based on the asymptotical approach to solving the scattering problem in a material with many small particles embedded in it help to understand better the dependence of the effective field in the material on the basic parameters of the problem, namely, on $a, M, d, \zeta_m, N(x), h(x)$.

It is shown that, for small number M of particles there is an optimal value of a, for which the relative error to asymptotic solution is minimal. When $a \to 0$ and M is small the matrix of (16) is diagonally dominant and the error goes to 0. This is confirmed by the numerical results as well. The relative error can be decreased by changing function $N(x)$ or by decreasing a, d being fixed, but the condition $d \gg a$ is not necessary to have if M is small.

The accuracy of the solution to the limiting equation (9) depends on the values of k, a, and on the function $h(x)$. The accuracy of the solution improves as the number P increases.

The relative error of the solution to asymptotic LAS (16) depends essentially on the function $N(x)$ which is at our disposal. In our numerical experiments $N(x) = const$. The accuracy of the solution is improved if $N(x)$ decreases. The error of the solution decreases if M grows.

The relative difference between the solutions to LAS (16) and (17) can be improved by changing the distance d between the particles, a being fixed. The optimal values of d change slowly in the considered range of function $N(x)$. The relative error is smaller for smaller a.

The constructive procedure for prescribing the function $N(x)$, calculating the numbers μ, and determining the radius a allows one to obtain the refraction coefficient approximating better the prescribed one.

These results help to apply the proposed technique for creating materials with a desired refraction coefficient using the recipe, formulated in this paper. Technological methods for embedding many small particles into a given domain D according to our recipe, and for preparing small balls with the desired large impedances $\zeta = \frac{h(x)}{a^\kappa}$ are two basic technological problems that should be solved for an immediate practical implementation of our recipe.

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