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A. G. Ramm, Scattering by many small inhomogeneities and applications

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Scattering by many small inhomogeneities and applications

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Abstract

Many-body quantum-mechanical scattering problem is solved asymptotically when the size of the scatterers (inhomogeneities) tends to zero and their number tends to infinity.

A method is given for calculation of the number of small inhomogeneities per unit volume and their intensities such that embedding of these inhomogeneities in a bounded region results in creating a new system, described by a desired potential. The governing equation for this system is a non-relativistic Schrödinger's equation described by a desired potential.

Similar ideas were developed by the author for acoustic and electromagnetic (EM) wave scattering problems.

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1 Introduction

In a series of papers, cited in the references, and in the monograph [8] the author has developed wave scattering theory by many small bodies of arbitrary shapes and, on this basis, proposed a method for creating materials with some desired properties, in particular, with a desired refraction coefficient. The goal of this paper is to describe a new method for creating materials with a desired refraction coefficient and to compare it with the method proposed earlier. The new method is applicable to the problems which deal with vector fields and tensorial refraction coefficients. Our presentation deals with the simpler case of scalar fields and uses paper [27].

Let us formulate the statement of the problem. Let $D \subset \mathbb{R}^3$ be a bounded domain filled in by a material with a known refraction coefficient. The scalar wave scattering problem consists of finding the solution to the Helmholtz equation:

$$L_0 u := [\nabla^2 + k^2 n_0^2(x)]u = 0 \quad \text{in} \quad \mathbb{R}^3, \quad \operatorname{Im} n_0^2(x) \geq 0, \tag{1}$$

$$u = u_0 + v, \quad u_0 := e^{ik\alpha\cdot x}, \tag{2}$$

$$v = A_0(\beta,\alpha)\frac{e^{ikr}}{r} + o(\frac{1}{r}), \quad r := |x| \to \infty, \quad \beta := \frac{x}{r}. \tag{3}$$

The function $n_0^2(x)$ is assumed bounded, Riemann-integrable,

$$n_0^2(x) = 1 \quad \text{in} \quad D' := \mathbb{R}^3 \backslash D, \quad \operatorname{Im} n_0^2(x) \geq 0. \tag{4}$$

The function $A(\beta,\alpha)$ is called the scattering amplitude. The wavenumber $k = \frac{2\pi}{\lambda}$, where λ is the wavelength in D', $\alpha \in S^2$ is the direction of the incident plane wave u_0, S^2 is the unit sphere in $\mathbb{R}^3$, $\beta \in S^2$ is the direction of the scattered wave. The solution to problem (1)-(3) is called the scattering solution. It is well-known ([5]) that this solution exists and is unique under our assumptions. These assumptions are: $n_0^2(x)$ is bounded: $\sup_{x\in\mathbb{R}^3} |n_0^2(x)| \leq n_0 = const$, $\operatorname{Im} n_0^2(x) \geq 0$, $n_0^2(x) = 1$ in D'. Since the solution u is unique, the corresponding scattering amplitude $A_0(\beta,\alpha)$ is determined uniquely if $n_0^2(x)$ is given. We assume $k > 0$ fixed and do not show the dependence of $A_0(\beta,\alpha)$ on k. The operator L_0 at a fixed $k > 0$ can be considered as a Schrödinger operator $L_0 = \nabla^2 + k^2 - q_0(x)$, where $q_0(x) := k^2 - k^2 n_0^2(x)$.

Problem RC:

We want to construct a material in D with a desired refraction coefficient, that is, with a desired function $n^2(x)$, $\operatorname{Im} n^2(x) \geq 0$.

Here RC stands for refraction coefficient.

Why is this problem of practical interest?

We give two reasons.

First, creating a refraction coefficient such that the corresponding material has *negative refraction* is of practical interest.

One says that a material has negative refraction if the group velocity in this material is directed opposite to the phase velocity.

Secondly, It is of practical interest to create a refraction coefficient such that the corresponding scattering amplitude $A(\beta) = A(\beta,\alpha)$ at a fixed $\alpha \in S^2$ (and a fixed $k > 0$) approximates an arbitrary given function $f(\beta) \in L^2(S^2)$ with any desired accuracy $\epsilon > 0$.

This problem we call *the problem of creating material with a desired wave-focusing property.*

In Section 2 we explain how to create a material with a desired refraction coefficient. In Section 3 we compare our recipe for creating material with a desired refraction coefficient with the recipe given in [24].

2 Creating material with a desired refraction coefficient by embedding small inhomogeneities into a given material

The basic idea of our method is to embed in D many small inhomogeneities $q_m(x)$ in such a way that the resulting medium can be described by a desired potential $q(x)$.

Let us assume that $p_M(x)$ is a real-valued compactly supported bounded function, which is a sum of small inhomogeneities:

$$p_M = \sum_{m=1}^{M} q_m(x),$$

where $q_m(x)$ vanishes outside the ball $B_m := \{x : |x - x_m| < a\}$ and $q_m = A_m$ inside B_m, $1 \leq m \leq M$, $M = M(a)$.

The question is:

Under what conditions the field u_M, which solves the Schrödinger equation with the potential $p_M(x)$, has a limit $u_e(x)$ as $a \to 0$, and this limit $u_e(x)$ solves the Schrödinger equation with a desired potential $q(x)$?

We give a complete answer to this question in Theorem 1 below.

The class of potentials q, that can be obtained by our method, consists of bounded, compactly supported, Riemann-integrable functions. It is known that the set of Riemann-integrable functions is precisely the set of almost everywhere continuous functions, that is, the set of bounded functions with the set of discontinuities of Lebesgue measure zero in $\mathbb{R}^3$. These assumptions on q are not repeated but are always valid when we write "an arbitrary potential".

In fact, a more general set of potentials can be constructed by our method. It is mentioned below that for some class of unbounded potentials, having local singularities, which are absolutely integrable, our theory remains valid.

Our result is as follows:

Assume that $q(x)$ is an arbitrary Riemann-integrable in D potential, vanishing outside D, where D is an arbitrary large but finite domain, and the functions $A(x)$ and $N(x)$, which we can choose as we wish, are chosen so that $A(x_m) = A_m$ and $A(x)N(x) = q(x)$, where $N(x) \geq 0$.

Then the limit $u_e(x)$ of $u_M(x)$ as $a \to 0$ does exist, and solves the scattering problem with the desired refraction coefficient $n^2(x)$:

$$\nabla^2 u_e + k^2 n^2(x) u_e := \nabla^2 u_e + k^2 u_e - q(x) u_e = 0, \tag{5}$$

$$u = u_0 + v, \tag{6}$$

where u_0 solves problem (5) and v satisfies the radiation condition.

The notation $u_e(x)$ stands for the effective field, which is the limiting field in the medium as $M \to \infty$, or, equivalently, $a \to 0$. Under our assumptions (see Lemma 1 below) one has $M = O(\frac{1}{a^3})$.

The field u_M is the unique solution to the integral equation:

$$u_M(x) = u_0(x) - \sum_{m=1}^{M} \int_D g(x,y,k) q_m(y) u_M(y) dy, \qquad g(x,y,k) = \frac{e^{ik|x-y|}}{4\pi|x-y|}, \tag{7}$$

where $u_0(x)$ is the incident field, which one may take as the plane wave, for example, $u_0 = e^{ik\alpha \cdot x}$, where $\alpha \in S^2$ is the direction of the propagation of the incident wave.

We assume that the scatterers are small in the sense $ka << 1$. Parameter $k > 0$ is assumed fixed, so the limits below are designated as limits $a \to 0$, and condition $ka << 1$ is valid as $a \to 0$.

If $ka << 1$, then the following transformation of (7) is valid:

$$u_M(x) = u_0(x) - \sum_{m=1}^{M} \frac{e^{ik|x-x_m|}}{4\pi} A_m u_M(x_m) \int_{|y-x_m|<a} \frac{dy}{|x-y|}[1+o(1)]. \tag{8}$$

To get (8) we have used the folowing estimates:

$$|x-x_m| - a \le |x-y| \le |x-x_m| + a, \qquad |y-x_m| \le a.$$

These estimates imply

$$e^{ik|x-y|} = e^{ik|x-x_m|}[1+o(1)],$$

provided that $|y-x_m| \le a$ and $a \to 0$.

We also have taken into account that, as $a \to 0$, one has:

$$\max_{x \in B_m} |u_M(x) - u_M(x_m)| = o(1).$$

A proof of this statement is given in [12].

Here is a sketch of another proof of the above statement. Equation (7) has a unique solution because it is an equation with a compactly supported bounded uniformly with respect to M potential p. Its solution satisfies a homogeneous Schrödinger equation and the radiation condition. Thus, this solution is unique. This solution is uniformly (with respect to M) continuous in D.

Yet another argument, different from the ones, given above, can be outlined as follows. The limiting funtion $u_e(x)$ is in $H^2(D)$ by the standard elliptic regularity results, so it is continuous in D. The function u_M converges to u_e uniformly. Therefore, it satisfies the above inequality as $M \to \infty$, or, equivalently, as $a \to 0$.

The fourth proof of the same statement can be based on a result from [26]. Namely, a justification of a collocation method for solving equation (17) (see below) for the limiting field u_e is given in [26]. From the arguments, given there, one obtains the uniform convergence of u_M to u_e:

$$\lim_{M \to \infty} \max_{x \in D} |u_M(x) - u_e(x)| = 0.$$

Let us return to equation (8).

We want to prove that the sum in (8) has a limit as $a \to 0$, and to calculate this limit assuming that the distribution of small inhomogeneities or, equivalently, the points x_m, is given by the following formula:

$$\mathcal{N}(\Delta) = |V(a)|^{-1} \int_{\Delta} N(x)dx[1+o(1)] \qquad a \to 0, \tag{9}$$

where $V(a) = 4\pi a^3/3$, $N(x) \ge 0$ is an arbitrary given function, continuous in the closure of D, $0 \le N(x) < \mathbf{p} < \mathbf{1}$, $\mathbf{p}$ is a constant arising in the problem of spheres packing, and $\mathcal{N}(\Delta)$ is the number of small inhomogeneities in an arbitrary open subset $\Delta \subset D$.

The maximal value of the constant constant $\mathbf{p}$ is the maximal ratio of the total volume of the packed spheres divided by $|\Delta|$, where $|\Delta|$ is the volume of Δ. The total volume of the balls, embedded in the domain Δ, is equal to

$$V_\Delta := V(a)\mathcal{N}(\Delta) = \int_\Delta N(x)dx[1 + o(1)].$$

If diam(Δ) is sufficiently small and $x \in \Delta$ is some point in Δ, then

$$V_\Delta = N(x)|\Delta|[1 + o(1)] < \mathbf{p}|\boldsymbol{\Delta}|.$$

Since the domain Δ is arbitrary, one lets $a \to 0$ and concludes that

$$N(x) \le \mathbf{p} < \mathbf{1}.$$

It is conjectured that maximal value of $\mathbf{p}$ *is equal approximately* 0.74. (see, e.g., [32]).

There is a large literature on optimal packing of spheres (see, e.g., [3], [32]). For us the maximal value of $\mathbf{p}$ is not important. What is important is the following conclusion:

One can choose $N(x) \ge 0$ as small as one wishes, and still create any desired potential $q(x)$ by choosing suitable $A(x) > 0$.

The total number $M = \mathcal{N}(D)$ of the embedded small inhomogeneities is $M = O(\frac{1}{a^3})$, according to (9).

Our basic new tool is the following lemma.

Lemma 1. *If the points x_m are distributed in a bounded domain $D \subset \mathbb{R}^3$ according to* (9)*, and $f(x)$ is an arbitrary Riemann-integrable in D function, then the following limit exists:*

$$\lim_{a\to 0} \sum_{m=1}^{M} f(x_m)V(a) = \int_D f(x)N(x)dx. \qquad (10)$$

The class of Riemann-integrable functions is precisely the class of bounded almost everywhere continuous functions, i.e., bounded functions with the set of discontinuities of Lebesgue measure zero in $\mathbb{R}^3$. The class of such functions is precisely the class of functions for which the Riemannian sums converge to the integrals of the functions.

The result in (10) we generalize to the class of functions for which the integral in the right-hand side of (10) exists as an improper integral. *In this case $f(x)$ may be unbounded at some points y*, but the limit $\lim_{\delta\to 0} \int_{D_\delta} f(x)N(x)dx$ exists and

$$\lim_{\delta\to 0} \int_{D_\delta} f(x)N(x)dx := \int_D f(x)N(x)dx,$$

where $D_\delta := D \setminus B(y, \delta)$, and $B(y, \delta)$ is the ball centered at $y \in D$ and of radius δ. In this case the sum in (10) is defined as follows:

$$\lim_{a\to 0} \sum_{m=1}^{M} f(x_m)V(a) := \lim_{\delta\to 0} \lim_{a\to 0} \sum_{x_m \in D_\delta} f(x_m)V(a). \qquad (11)$$

The same definition is valid for the conclusion of Theorem 1, which is our result.

Theorem 1. *If the small inhomogeneities are distributed so that* (9) *holds, and* $q_m(x) = 0$ *if* $x \notin B_m$, $q_m(x) = A_m$ *if* $x \in B_m$, *where* $B_m = \{x : |x - x_m| < a\}$, $A_m := A(x_m)$, *and* $A(x)$ *is a given in* D *function such that the function* $q(x) := A(x)N(x)$ *is Riemann-integrable, then the limit*

$$\lim_{a \to 0} u_M(x) = u_e(x) \tag{12}$$

does exist and solves problem (5)-(6) *with the potential*

$$q(x) = A(x)N(x). \tag{13}$$

There is a large literature on wave scattering by small inhomogeneities. A recent paper, which we use, is [27]. Some of the ideas of this approach were earlier applied by the author to scattering by small particles embedded in an inhomogeneous medium (see [3]-[23]).

We apply Lemma 1 to the sum in (8), in which we choose $A_m := A(x_m)$, where $A(x)$ is an arbitrary continuous in D function which we may choose as we wish. A simple calculation yields the following formulas:

$$\int_{|y-x_m|<a} |x-y|^{-1}dy = V(a)|x-x_m|^{-1}, \qquad |x-x_m| \geq a, \tag{14}$$

and

$$\int_{|y-x_m|<a} |x-y|^{-1}dy = 2\pi(a^2 - \frac{|x-x_m|^2}{3}), \qquad |x-x_m| \leq a. \tag{15}$$

Therefore, the sum in (8) is of the form (10) with

$$f(x_m) = \frac{e^{ik|x-x_m|}}{4\pi|x-x_m|}A(x_m)u_M(x_m)[1+o(1)]. \tag{16}$$

Applying Lemma 1, one concludes that the limit $u_e(x)$ in (12) does exist and solves the integral equation

$$u_e(x) = u_0(x) - \int_D \frac{e^{ik|x-y|}}{4\pi|x-y|}q(y)u_e(y)dy, \tag{17}$$

where $q(x)$ is defined by formula (13).

Applying the operator $\nabla^2 + k^2$ to (17), one verifies that the function $u_e(x)$ solves problem (5)-(6).

Thus, the conclusion of Theorem 1 is established.

In (16) $f(x_m)$ depends on a through $u_M(x_m)$. Nevertheless Lemma 1 is applicable because $u_M(x)$ converges to the solution $u_e(x)$ of eqution (17) as $a \to 0$. This follows from the results in [26] and [12]. These results give two independent ways to prove convergence of u_M to u_e as $a \to 0$. The results in [12] yield compactness of the set $\{u_M(x)\}$, while the results in [26] convergence of a version of the collocation method for solving equation

(17) is proved. This version of the collocation method leads to solving the following linear algebraic system

$$u_j = u_{0j} - \sum_{m=1, m\neq j}^{n} g_{jm} q_m u_m V(a), \quad 1 \leq j \leq m, \tag{18}$$

where $u_j := u(x_j)$, $q_m := q(x_m)$, and $g_{jm} := \frac{e^{ik|x_j - x_m|}}{4\pi|x_j - x_m|}$. It is proved in [26] that the linear algebraic system (18) has a solution and this solution is unique for all sufficiently small a, and the function

$$u^{(n)}(x) := \sum_{m=1}^{n} u_j \chi_j(x)$$

converges to $u_e(x)$ uniformly:

$$\lim_{n\to\infty} ||u_e(x) - u^{(n)}(x)||_{C(D)} = 0,$$

where $\chi_j(x) = 1 \quad x \in D$, $\chi_j(x) = 0 \quad x \notin D$.

In particular, it is proved in [26] that a collocation method for solving equation (17) leads to sums, similar to the sum on the left-hand side of (10), and the collocation method, studied in [26], converges to the unique solution of the equation (17). This means that the function $u_M(x)$ converges to $u_e(x)$.

Remark 1. The quantities A_m in the definition of q_m can be it tensors. In this case *the refraction coefficient* $n^2(x)$ *of the created material is a tensor, and* u *is a vector field.*

Remark 2. The recipe for creating materials with the desired refraction coefficient by the method, based on Theorem 1, can be summarized as follows:

Recipe 1: Given a bounded domain filled with the material with the refraction coefficient $n_0^2(x)$*, one embeds the small inhomogeneities* q_m*,* $q_m = 0$ *for* $|x - x_m| > a$*,* $q_m = A_m := A(x_m)$*, where the points* x_m *are distributed by the rule* (9)*, and one chooses* $A(x)$ *and* $N(x) \geq 0$*, so that* $A(x)N(x) = q(x)$*, where* $q(x)$ *is the desired potential, or which is the same, the desired refraction coefficient* $n^2(x) := 1 - k^{-2}q(x)$*. The material, created by the embedding of these small inhomogeneities, in the limit* $a \to 0$*, has the refraction coefficient* $n^2(x) = 1 - k^{-2}q(x)$*.*

One can fix $N(x) \geq 0$ *and choose* $A(x)$ *such that the function* $q(x) = A(x)N(x)$ *is a desired function, so that* $n^2(x) = 1 - k^{-2}q(x)$ *is a desired function.*

We call this recipe *Recipe i*, where *i* stands for inhomogeneities.

3 A discussion of two recipes

In [24] a different recipe was proposed for creating materials with a desired refraction coefficient. We call the recipe from [24] *Recipe p*, where *p* stands for particles. *Recipe p* consists of embedding small particles, for example, balls of radius a, $ka << 1$, into a given material according to the distribution law, similar to the one in (9), but with $a^{2-\kappa}$ in place of $V(a)$, where $\kappa \in (0, 1]$ is a parameter experimenter can choose at will. The physical properties of the embedded particles are described by the boundary impedance

$\zeta_m = \frac{h(x_m)}{a^{\varkappa}}$. The function $h(x)$, determining the boundary impedances, can also be chosen as one wishes. We refer the reader to the paper [24] for details. Numerical results on the implementation of *Recipe p* are given in [2] and [4].

There are two technological problems that should be solved in order that *Recipe p* be implemented practically.

Technological Problem 1: *How does one embed many small particles in a given material so that the desired distribution law is satisfied?*

Technological Problem 2: *a) How does one prepare a small particle with the desired boundary impedance* $\zeta_m = \frac{h(x_m)}{a^{\varkappa}}$*?*

b) How can one prepare a small particle with the desired dispersion of the boundary impedance, that is, the desired ω*-dependence of* $h = h(x, \omega)$*?*

The motivation for the last question is the following: by creating material with the refraction coefficient depending on the frequency ω in a desired way, one can, for instance, prepare materials with negative refraction.

The first problem, possibly, can be solved by *stereolitography.*

The second problem one should be able to solve because the limiting cases $\zeta_m = 0$ (hard particles) and $\zeta_m = \infty$ (soft particles) can be prepared, so that any intermediate value of ζ_m one should be able to prepare as well.

The author formulates the above technological problems in the hope that engineers get interested and solve them practically.

In *Recipe p* the number M of the embedded particles is $M := M_2 = O(\frac{1}{a^{2-\kappa}})$, while in *Recipe i* the number M is $M := M_1 = O(\frac{1}{a^3})$. Thus, $M_1 >> M_2$ as $a \to 0$. So, in recipe 2 one has to embed much smaller number of small particles than in *Recipe i*. This is an advantage of *Recipe p* over *Recipe i*. The disadvantage of *Recipe p*, compared with *Recipe i*, is in the possible practical difficulties of creating particles with the prescribed very large boundary impedances $\zeta_m = O(\frac{1}{a^{\kappa}})$ when a is very small.

3.1 Negative refraction

Material with negative refraction is, by definition, a material in which group velocity is directed opposite to the phase velocity, (see [1] and references therein). Group velocity is defined by the formula $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega(\mathbf{k})$. Phase velocity $\mathbf{v}_p$ is directed along the wave vector $\mathbf{k}^0 = \frac{\mathbf{k}}{|\mathbf{k}|}$. In an isotropic material $\omega = \omega(|\mathbf{k}|)$, and $\omega n(x, \omega) = c|\mathbf{k}|$. Differentiating this equation yields

$$\nabla_{\mathbf{k}}\omega\big[n(x,\omega) + \omega\frac{\partial n}{\partial \omega}\big] = c\mathbf{k}^0. \tag{19}$$

Thus,

$$\mathbf{v}_g\big[n + \omega\frac{\partial n}{\partial \omega}\big] = c\mathbf{k}^0. \tag{20}$$

Wave speed in the material is $|\mathbf{v}_p| = \frac{c}{n(x,\omega)}$, where c is the wave speed in vacuum (in D'), and $n(x, \omega)$ is a scalar, and $\mathbf{v}_p$ is directed along $\mathbf{k}^0$.

For $\mathbf{v}_g$ to be directed opposite to $\mathbf{v}_p$ it is necessary and sufficient that

$$n + \omega\frac{\partial n}{\partial \omega} < 0. \tag{21}$$

If the new material has the function $n(x, \omega)$ satisfying (21), then the new material has negative refraction.

One can create material with the refraction coefficient $n^2(x, \omega)$ having a desired dispersion, i.e., a desired frequency dependence, by choosing function $h = h(x, \omega)$ properly.

Let us formulate the technological problem solving of which allows one to implement practically *Recipe p* for creating materials with negative refraction.

Technological Problem 3: *How does one prepare a small particle with the desired frequency dependence of the boundary impedance* $\zeta_m = \frac{h(x_m, \omega)}{a^\kappa}$, *where* $h(x, \omega)$ *is a given function?*

This problem is the same as *Technological Problem 2b)*, formulated above.

3.2 Wave-focusing property

Let us formulate the problem of preparing a material with a desired wave-focusing property. The refraction coefficient is related to the potential by the formula

$$q(x) = k^2 - k^2 n^2(x).$$

We assume in this Section that $k > 0$ is fixed, and $\alpha \in S^2$, the incident direction (that is, the direction α of the incident plane wave $e^{ik\alpha\cdot x}$) is also fixed.

Problem: Given an arbitrary fixed $f(\beta) \in L^2(S^2)$, *an arbitrary small fixed* $\epsilon > 0$, *an arbitrary fixed* $k > 0$, *and an arbitrary fixed* $\alpha \in S^2$, *can one find* $q \in L^2(D)$, $q = 0$ *in* $D' = R^3 \backslash D$, *such that*

$$\|A_q(\beta) - f(\beta)\|_{L^2(S^2)} < \epsilon, \tag{22}$$

where $A_q(\beta) := A_q(\beta, \alpha, k)$ *is the scattering amplitude, corresponding to* q, *at fixed* α *and* k, *and* $q := k^2 - k^2 n^2(x)$*?*

The answer is *yes*, and an algorithm for finding such a q, and, therefore, such an $n^2(x)$, is given in [17]. See also [18], [20]. The above problem is the inverse scattering problem with the scattering data given at a fixed k and a fixed direction α of the incident plane wave.

There are many potentials q which solve the above problem. It is possible to choose from the set of these potentials the one which satisfies some additional properties, for example, one can choose q to be arbitrarily smooth in D, one can try to choose q with non-negative imaginary part, etc.

The desired radiation pattern $f(\beta)$ can, for example, be equal to 1 in a given solid angle and equal to 0 outside this solid angle. In this case the scattered field is scattered predominantly into the desired solid angle.

This is why we call such a material a material with wave-focusing property.

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