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Scattering by many small bodies and applications to condensed matter physics

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Abstract

Equations for the effective field in the medium, in which many small particles are embedded, are derived. It is shown how to create a material with a desired refraction coefficient by embedding in a given material many small particles.

1 Introduction and statement of the results

Let $D \subset \mathbb{R}^3$ be a bounded domain with a boundary S , filled with a material whose refraction coefficient $n_0^2(x)$ is known, $x \in \mathbb{R}^3$. The scattering problem consists of solving the equation:

$$L_0 u_0 := [\nabla^2 + k^2 n_0^2(x)] u_0 = 0 \quad \text{in } \mathbb{R}^3, \quad u_0 = e^{ik\alpha \cdot x} + v_0, \quad (1)$$

where $k > 0$ is fixed, $\alpha \in S^2$ is a unit vector in the direction of the incident wave, $n_0^2 = 1$ in $D' = \mathbb{R}^3 \setminus D$, v_0 is the scattered field satisfying the radiation condition:

$$\partial v_0 / \partial r - ik v_0 = o(r^{-1}), \quad r := |x| \rightarrow \infty. \quad (2)$$

One can write $L_0 = \nabla^2 + k^2 - q_0(x)$, $q_0(x) := k^2[1 - n_0^2(x)]$, $q_0 = 0$ in D' . The k -dependence in $q_0(x)$ is not shown because k is fixed. Let $G(x, y)$ be the resolvent kernel of L_0 : $L_0 G = -\delta(x - y)$, $\delta(x)$ is the delta-function, G satisfies the radiation condition. Assume that $M \gg 1$ small particles D_m are embedded into D , $a := \frac{1}{2} \max_{1 \leq m \leq M} \text{diam } D_m$, $n_0 k a \ll 1$, $n_0 = \max_{x \in \mathbb{R}^3} |n_0(x)|$, $d =$

$\min \text{dist}_{m \neq j}(D_m, D_j)$, $d \gg a$. Since $q_0(x)$ is known, we assume that $G(x, y)$ and $u_0(x)$ are known. Consider the scattering problem:

$$L_0 u_M = 0 \quad \text{in } \mathbb{R}^3 \setminus \bigcup_{m=1}^M D_m, \quad u_M = u_0 + v_M, \quad (3)$$

$$\frac{\partial u_M}{\partial N} = \zeta_m u_M \quad \text{on } S_m, \quad 1 \leq m \leq M, \quad (4)$$

where S_m is the boundary of D_m , N is the unit normal to S_m pointing out of D_m , ζ_m is the boundary impedance, v_M satisfies the radiation condition. We assume that S_m are sufficiently smooth, e.g., $S_m \in C^{1,\lambda}$, $\lambda > 0$, uniformly in m , and

$$\text{Im } q_0(x) \leq 0, \quad \text{Im } \zeta_m \leq 0. \quad (5)$$

One can prove that problem (3), (4) has a unique solution under these assumptions, and this solution is of the form:

$$u_M = u_0(x) + \sum_{m=1}^M \int_{S_m} G(x, s) \sigma_m(s) ds, \quad (6)$$

where the functions σ_m are to be chosen so that conditions (4) are satisfied. Let $Q_m := \int_{S_m} \sigma_m(s) ds$. Write (6) as

$$u_M = u_0 + \sum_{m=1}^M G(x, x_m) Q_m + \sum_{m=1}^M \int_{S_m} [G(x, s) - G(x, x_m)] \sigma_m(s) ds, \quad x_m \in D_m. \quad (7)$$

Since D_m are small, the choice of $x_m \in D$ is not important. If $|x - x_m| \geq d \gg a$, $|\zeta_m| = O(a^{-1})$, $1 \leq m \leq M$, then, as we show, the second sum in (7) is negligible compared with the first, and one can write

$$u_M = u_0 + \sum_{m=1}^M G(x, x_m) Q_m + O\left(\frac{a}{d}\right), \quad |x - x_m| \geq d \gg a. \quad (8)$$

Our aims are: 1) to derive a formula for Q_m , 2) to pass to the limit $M \rightarrow \infty$ in (8) and to obtain an equation for the effective field $\mathcal{U}(x)$ in the region filled with many small particles, 3) to give a method for creating a "smart" material with a desired refraction coefficient $n^2(x)$ by embedding into D many small particles: we give a formula for the number $a^{-1} \mathcal{N}(x) dx$ of particles to be embedded in a volume dx around a point x , and for their impedances $\zeta(x)$, given the desired refraction coefficients $n^2(x)$ and $n_0^2(x)$.

There is a large literature on wave scattering by small particles. The theory was originated by Rayleigh (1871), who studied wave scattering by a single small particle and showed that the main contribution to the scattered field comes from

the dipole radiation. The smallness of the particle allows one to consider the incident field as a constant field, to solve the static problem, to find the induced dipole moment P , and to calculate the corresponding scattered field ([1], §72). Rayleigh did not give formulas for calculating P for particles (small bodies) of arbitrary shapes. This was done by the author (see [4] and references therein). In [4] formulas for electric and magnetic polarizability tensors are derived. In [2] boundary-value problems are studied in domains with boundaries consisting of many small components on which the Dirichlet condition holds, and the operators are elliptic selfadjoint and positive, e.g., Laplace operator. The arguments in [2] do not seem to be applicable to our problem because our operator is not positive-definite, it may be nonselfadjoint if $n_0^2(x)$ is a complex-valued function, which corresponds to an absorption, and we use impedance boundary conditions not considered in [2]. It is these conditions that allow us to create materials with arbitrary refraction coefficients. In the case of Neumann boundary condition the Helmholtz operator is considered in [2]. We use some ideas from [5]–[8].

Let $\mathcal{J}_m := \int_{S_m} \int_{S_m} \frac{ds dt}{|s-t|}$, $V_m = |D_m|$ be the volume of D_m , $|S_m|$ be the surface area of S_m , $\beta_{pj}^{(m)}$ be the magnetic polarizability tensor of D_m , defined in [4], p. 62, formula (5.62), (see also [3], pp 383–384). Let $\tilde{D} \subset D$ be an arbitrary subdomain of D . Assume that

$$M = O(a^{-1}), \quad d = O(a^{1/3}), \quad |S_m| = c_1 a^2, \quad \mathcal{J}_m = c_2 a^3, \quad V_m = c_3 a^3. \quad (9)$$

These assumptions can be relaxed: the constants c_j , $1 \leq j \leq 3$, may depend on m , but we do not go into detail. What is important for our arguments is the order of $M, d, S_m, \mathcal{J}_m$ and V_m as $a \rightarrow 0$. Assumptions (9) hold in Theorem 1. In Theorem 2 the assumptions $M = O(a^{-1})$, $d = O(a^{1/3})$ are no longer valid.

The continuous functions $h(x)$ and $\mathcal{N}(x)$ in Theorem 1 and $\nu(x)$ in Theorem 2 are independent of a and can be chosen a priori. The subdomains $\tilde{D}$ in Theorems 1 and 2 are arbitrary subdomains of D independent of a . Let

$$N_a(\tilde{D}) := \sum_{D_m \subset \tilde{D}} 1$$

be the number of particles in $\tilde{D}$. This number grows to infinity as $a \rightarrow 0$, provided that $\int_{\tilde{D}} \mathcal{N}(x) dx > 0$.

The function $h(x)$ defines the boundary impedances of the particles near a point $x \in D$.

The function $\mathcal{N}(x)$ defines the number of small particles in $\tilde{D}$ by the equation (11) in Theorem 1.

The assumption (10) in Theorem 1 means that the small particle D_m shrinks to a point $x \in D$, independent of m , as $a \rightarrow 0$. For this reason we do not write x_m in place of x .

Let us now formulate our results.

Theorem 1 Assume that

$$\lim_{a \rightarrow 0} \frac{\zeta_m \mathcal{J}_m}{4\pi |S_m|} = h(x), \quad x \in D_m, \quad (10)$$

$$\lim_{a \rightarrow 0} a N_a(\tilde{D}) = \int_{\tilde{D}} \mathcal{N}(x) dx. \quad (11)$$

Then there exists $\lim_{M \rightarrow \infty} u_M = \mathcal{U}(x)$, the function $\mathcal{U}(x)$ solves the equation

$$L\mathcal{U} := [\nabla^2 + k^2 - q(x)]\mathcal{U} = 0 \quad \text{in } \mathbb{R}^3, \quad q(x) := q_0(x) + p(x), \quad (12)$$

$$p(x) := \frac{4\pi c_1^2}{c_2} \frac{\mathcal{N}(x)h(x)}{1 + h(x)}, \quad (13)$$

where $c_1, c_2 > 0$ are the constants from (9), $\mathcal{N}(x)$ is the function from (11), and $h(x)$ is the function from (10). The function $\mathcal{U} = u_0 + V$, where V satisfies the radiation condition. The scattering amplitude, corresponding to $q(x)$, is:

$$A(\beta, \alpha) = A_0(\beta, \alpha) - \frac{1}{4\pi} \int_D u_0(y, -\beta) p(y) \mathcal{U}(y, \alpha) dy, \quad (14)$$

where $A_0(\beta, \alpha)$ is the scattering amplitude corresponding to $q_0(x)$, and $u_0(x, \beta)$ is the scattering solution, corresponding to $q_0(x)$. One has:

$$\mathcal{U}(x, \alpha) = e^{ik\alpha \cdot x} + A(\beta, \alpha) \frac{e^{ikr}}{r} + o\left(\frac{1}{r}\right), \quad r = |x| \rightarrow \infty, \quad \beta := \frac{x}{r}. \quad (15)$$

Remark 1 Under the assumptions (9) – (10) one has

$$\zeta_m = \frac{4\pi c_1}{c_2 a} h(x) \quad \text{as } a \rightarrow 0, \quad x \in D_m. \quad (16)$$

Theorem 2 Assume that $\zeta_m = 0$, $1 \leq m \leq M$, $d \gg a$, and the following limits exist:

$$\lim_{a \rightarrow 0} \sum_{D_m \subset \tilde{D}} V_m \beta_{pj}^{(m)} = \int_{\tilde{D}} \beta_{pj}(y) \nu(y) dy, \quad \lim_{a \rightarrow 0} \sum_{D_m \subset \tilde{D}} V_m = \int_{\tilde{D}} \nu(y) dy, \quad (17)$$

where $\nu(y) \geq 0$ and $\beta_{pj}(y)$ are continuous functions in D and $\tilde{D}$ is an arbitrary subdomain of D . Then there exists the function $\mathcal{U}(x) := \lim_{M \rightarrow \infty} u_M(x)$, where $u_M(x)$ is defined in (6), and $\mathcal{U}(x)$ solves the equation

$$\mathcal{U}(x) = u_0(x) + \int_D G(x, y) \Delta \mathcal{U}(y) \nu(y) dy - \sum_{p,j=1}^3 \int_D \frac{\partial G(x, y)}{\partial y_p} \frac{\partial \mathcal{U}(y)}{\partial y_j} \beta_{pj}(y) \nu(y) dy. \quad (18)$$

Example 1 Under the assumptions of Theorem 1, let all the particles be balls of radius a . Then $|S_m| = 4\pi a^2$, $\mathcal{J}_m = 16\pi^2 a^3$, $4\pi c_1/c_2 = 1$, $p(x) = 4\pi\mathcal{N}(x)h(x)[1 + h(x)]^{-1}$ by formula (13), the limit (10) exists iff $\zeta_m = h(x)a^{-1}$, where $x \in D_m$, and $\mathcal{N}(x)|\Delta_x| = aN(\Delta_x)$, where Δ_x is a small cube centered at x and $N(\Delta_x)$ is the number of small balls of radius a in Δ_x . Given an arbitrary continuous function $n^2(x)$, $\text{Im } n^2(x) \geq 0$, one calculates $q(x) = k^2[1 - n^2(x)]$, $p(x) = k^2[n_0^2(x) - n^2(x)]$, and then finds the three functions $\mathcal{N}(x) \geq 0$, $h_1(x)$ and $h_2(x) \leq 0$, $h(x) := h_1(x) + ih_2(x)$, such that

$$p(x) = 4\pi\mathcal{N}(x)h(x)[1 + h(x)]^{-1}. \quad (*)$$

The function $p(x) = p_1(x) + ip_2(x)$ satisfies the condition $p_2(x) \leq 0$, which means that absorption in the medium is nonnegative. There are many ways to choose $\mathcal{N}(x) \geq 0$, $p_1(x)$ and $p_2(x) \leq 0$, so that $(*)$ holds. For example, if $p_1(x) > 0$, $p_2 \neq 0$, one may take $h_1(x) = 0$, $h_2(x) = \frac{p_1(x)}{p_2(x)}$, $\mathcal{N}(x) = \frac{p_1^2(x) + p_2^2(x)}{4\pi p_1(x)}$. Let us take $\tilde{D} = \Delta_x$ and embed in the small cube Δ_x with the side of length $b = 10^{-2}\text{cm}$ the small balls of radius $a = 10^{-5}\text{cm}$ with $d = 10^{-3}\text{cm}$. There will be $(\frac{b}{d})^3 = 10^3$ small balls in Δ_x , the assumption $d \gg a$ is satisfied, condition (11) implies $10^3 = 10^5\mathcal{N}(x)(10^{-2})^3$, i.e., $\mathcal{N}(x) = 10^4$.

One can create a material with any desirable refraction coefficient $n^2(x)$ by embedding into D small balls with the number of balls in a small cube Δ_x , centered at a point $x \in D$, calculated by formula (11) and their surface impedances $h(x)$ calculated by formula (10). The functions $\mathcal{N}(x)$ and $h(x)$ are calculated from the given $n^2(x)$. We have explained in Example 1 how to calculate $\mathcal{N}(x)$ and $h(x)$ given $n^2(x)$.

In Section 2 a brief outline of the derivations of the results is given.

2 Outline of proof

Proof of Theorem 1. To derive a formula for the numbers Q_m in (8), use the boundary condition (4) and get the following equation:

$$0 = u_{eN} - \zeta_j u_e + \frac{A_j \sigma_j - \sigma_j}{2} - \zeta_j T_j \sigma_j \quad \text{on } S_j, \quad 1 \leq j \leq M, \quad (19)$$

where u_e is the effective field, acting on the j -th particle,

$$\begin{aligned} T_j \sigma_j &:= \int_{S_j} G(s, t) \sigma_j(t) dt, \quad A_j \sigma_j = 2 \int_{S_j} \frac{\partial G(s, t)}{\partial N_s} \sigma_j(t) dt, \\ u_e(s) &:= u_M(s) - \int_{S_j} G(s, t) \sigma_j(t) dt. \end{aligned} \quad (20)$$

We prove that $G(x, y) = g_0(x, y)[1 + O(|x - y|)]$ as $|x - y| \rightarrow 0$, where $g_0 := (4\pi|x - y|)^{-1}$. Thus, we can replace G by g_0 in T_j and in A_j . Then we use

the relation $\int_{S_j} A_j \sigma_j ds = - \int_{S_j} \sigma_j ds$, see [4], p.96, formula (7.21). Integrating (19) over S_j we derive after some calculations (see [4], p.97, formula (7.26)), the following equation:

$$Q_j = - \frac{\zeta_j |S_j|}{1 + \zeta_j \mathcal{J}_j(4\pi |S_j|)^{-1}} u_e(x_j). \quad (21)$$

This and (8) imply

$$u_M = u_0 - \sum_{m=1}^M G(x, x_m) \frac{4\pi c_1^2 h(x_m) a}{c_2 [1 + h(x_m)]} u_e(x_m). \quad (22)$$

To pass to the limit $M \rightarrow \infty$, i.e., $a \rightarrow 0$, in (22), we use (10) and (11) and get

$$\mathcal{U}(x) = u_0(x) - \int_D G(x, y) p(y) \mathcal{U}(y) dy. \quad (23)$$

Applying the operator L_0 to (23) and using the equation $L_0 G = -\delta(x - y)$, one gets equation (12), and formula (13) for $p(x)$.

Clearly $\mathcal{U}$ satisfies the radiation condition (15). Formula (14) follows from (23) and the author's lemma (see [3], p. 257, formula (5.17)). In the limit $a \rightarrow 0$ there is no difference between $\lim_{a \rightarrow 0} u_e(x)$ and $\lim_{a \rightarrow 0} u_M(x)$.

Outline of the proof of Theorem 2. The principal novelty from the physical viewpoint is that if $\zeta_m = 0 \forall m$, then the second sum in (7) is of the same order of magnitude as the first (it can be even larger than the first). Therefore, now the second term in (7) cannot be neglected, in contrast to the case considered in Theorem 1. In place of equation (19), now one gets:

$$0 = u_{eN} + \frac{A_j \sigma_j - \sigma_j}{2}. \quad (24)$$

Integrating this equation over S_j , one gets

$$Q_j = \int_{S_j} u_{eN} dx = \int_{D_j} \Delta u_e dx \simeq \Delta u_e(x_j) V_j.$$

Thus, now $Q_j = O(k^2 a^3)$, while under the assumptions of Theorem 1 we had $Q_j = O(a)$. Since $ka \ll 1$, the quantity Q_j is now much smaller than in Theorem 1. Let us show that the integral

$$I_j := \int_{S_j} [G(x, s) - G(x, x_j)] \sigma_j(s) ds$$

is of the same order of magnitude as Q_j .

We have $G(x, s) - G(x, x_m) = \nabla_y G(x, y)|_{y=\tilde{y}} \cdot (s - x_m)$, where $\tilde{y}$ is some point of the segment (x_m, s) . If $|x - x_j| \geq d \gg a$, and a is very small, then $\nabla_y G(x, \tilde{y}) \simeq \nabla_y G(x, x_j)$. Thus,

$$I_j = \frac{\partial G(x, x_j)}{\partial y_p} \int_{S_j} (s - x_j)_p \sigma_j(s) ds,$$

where over the repeated index p one sums up, and $(s - x_j)_p$ is the p -th coordinate of the vector $s - x_j$. The integral in I_j is calculated using formulas (5.61), and (5.62), in [4], p.62. The result is:

$$\int_{S_j} (s - x_j)_p \sigma_j(s) ds = -V_j \frac{\partial u_e(x_j)}{\partial y_\ell} \beta_{p\ell}^{(j)}, \quad (25)$$

where $\beta_{p\ell}^{(j)}$ is the magnetic polarizability tensor defined in [4], p. 62, V_j is the volume of D_j , and over the repeated index ℓ (but not over j) one sums up. The quantity $I_j = O(k^2 a^3)$, i.e., it is of the same order as Q_j . Indeed, $V_j = O(a^3)$, and two differentiations with respect to y_p and y_ℓ bring the factor k^2 . Thus

$$u_M(x) = u_0(x) + \sum_{m=1}^M G(x, x_m) \Delta u_e(x_j) V_j - \sum_{m=1}^M \sum_{p,\ell=1}^3 \frac{\partial G(x, x_m)}{\partial y_p} V_m \frac{\partial u_e(x_m)}{\partial y_\ell} \beta_{p\ell}^{(j)}. \quad (26)$$

Passing to the limit $M \rightarrow \infty$, $a \rightarrow 0$, and using (7), one obtains equation (18). The existence of the second limit (17) is compatible with the assumption $d \gg a$ only if $\nu(y)$ is very small. Indeed, the second equation (17) implies that $\nu(y) = O(a^3 d^{-3})$.

If $\nu(y)$ and $\nabla \nu(y)$ are very small, then the first approximation to the solution of equation (18) is given by the formula

$$\mathcal{U}(x) = u_0(x) + \int_D G(x, y) \Delta u_0 \nu(y) dy - \sum_{p,j=1}^3 \int_D \frac{\partial G(x, y)}{\partial y_p} \frac{\partial u_0(y)}{\partial y_j} \beta_{pj}(y) \nu(y) dy. \quad (27)$$

In general, equation (18) is not local, it is an integral-differential equation. If one assumes that $\nu(y)|_S = 0$, then one can integrate by parts the last integral in (18) and get an equation from which a differential equation can be derived:

$$\mathcal{U}(x) = u_0(x) + \int_D G(x, y) \left[\nu(y) \Delta \mathcal{U}(y) + \sum_{p,j=1}^3 \frac{\partial}{\partial y_p} \left(\frac{\partial \mathcal{U}(y)}{\partial y_j} \beta_{pj}(y) \nu(y) \right) \right] dy. \quad (28)$$

Applying the operator L_0 to (28) one gets a differential equation:

$$L_0 \mathcal{U} + \nu(y) \Delta \mathcal{U} + \sum_{p,j=1}^3 \frac{\partial}{\partial y_p} \left(\frac{\partial \mathcal{U}(y)}{\partial y_j} \beta_{pj}(y) \nu(y) \right) = 0. \quad (29)$$

In [9] one finds detailed proofs.

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