Homogenization of a thin layer of randomly distributed nano-particles : effective model and error estimates

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Abstract

We study the time-harmonic scattering by a heterogeneous object covered with a thin layer of randomly distributed nanoparticles. We propose, via a multi-scale asymptotic expansion of the solution, an effective model where the layer of particles is replaced by an equivalent boundary condition. Under the assumption that the particles are distributed given a stationary and ergodic random point process, we prove that the so-called corrector problems are well-posed and establish quantitative error estimates between the original and effective solutions.

Keywords: Stochastic homogenization

1 Introduction

Let us consider an infinite plane, denoted $\Sigma_0 := \{x_d = 0\}$, covered by a thin layer of width εh_L of randomly distributed particles $\mathcal{P}^\omega_\varepsilon$ of size ε. Let $D^\omega_\varepsilon := \mathbb{R}^{d-1} \times \mathbb{R}^+ \setminus \bar{\mathcal{P}}^\omega_\varepsilon$ be the half space above Σ_0 outside the particles $\mathcal{P}^\omega_\varepsilon$ for a given distribution.

For a given source function $f \in L^2(D^\omega_\varepsilon)$ whose support lies far away from the layer, we look for the solution u^ω_ε of the Helmholtz equation

$$-\Delta u^\omega_\varepsilon - k^2 u^\omega_\varepsilon = f \quad \text{in } D^\omega_\varepsilon$$

where k is the wavenumber. The infinite plane models a multilayer object through a Robin boundary condition

$$\nabla u^\omega_\varepsilon \cdot \mathbf{e}_d = \gamma u^\omega_\varepsilon \quad \text{on } \Sigma_0,$$

where $\gamma \in \mathbb{C}$ is such that $\mathrm{Im}\,[\gamma] > 0$. At the boundary of the particles $\partial\bar{\mathcal{P}}^\omega_\varepsilon$, we impose to the field either a homogeneous Dirichlet condition

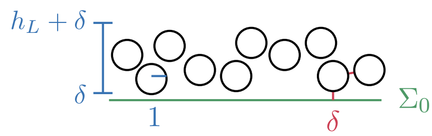
$$u^\omega_\varepsilon = 0 \quad \text{on } \partial\mathcal{P}^\omega_\varepsilon$$

or a homogeneous Neumann boundary condition

$$\nabla u^\omega_\varepsilon \cdot n = 0 \quad \text{on } \partial\mathcal{P}^\omega_\varepsilon.$$

Finally, the problem formulation has to be completed by a radiation condition.

Let L denote the infinite strip $L := \mathbb{R}^{d-1} \times [\delta, h_L + \delta]$ where $\delta > 0$. Let $\{\boldsymbol{x}_n\}^\omega_n$ denote the point process corresponding to the centers of the particles. Let $B(x^\omega_n)$ be the particle with radius 1 centered at x^ω_n. We suppose that $\{\boldsymbol{x}_n\}^\omega_n$ is stationary and ergodic and that the particles lie in L at least at a distance of δ from one another. We introduce $\mathcal{P}^\omega := \bigcup_n B(\boldsymbol{x}^\omega_n)$ the set of particles in L and $\mathcal{P}^\omega_\varepsilon := \bigcup_n \varepsilon B(\boldsymbol{x}^\omega_n)$ the set of particles of size ε in the rescaled strip $L^\varepsilon := \varepsilon L$.



2 A formal asymptotic expansion

Let $D^\omega_{\varepsilon H} := \mathbb{R}^{d-1} \times (0, \varepsilon H) \setminus \bar{\mathcal{P}}^\omega_\varepsilon$ and $D_{\varepsilon H,\infty} := \mathbb{R}^{d-1} \times [\varepsilon H, +\infty)$ for a given $H > 0$.

We propose the following Ansatz for u^ω_ε :

$$\begin{aligned} u^\omega_\varepsilon(\boldsymbol{x}) &= \sum_{n\in\mathbb{N}} \varepsilon^n \left[U^{\omega,NF}_n\left(\boldsymbol{x}_{\shortparallel}; \frac{\boldsymbol{x}_{\shortparallel}}{\varepsilon}, \frac{x_d}{\varepsilon}\right) + u^{\omega,FF}_n(\boldsymbol{x})\right] \quad \text{in } D_{\varepsilon H,\infty} \\ &= \sum_{n\in\mathbb{N}} \varepsilon^n\, U^{\omega,NF}_n\left(\boldsymbol{x}_{\shortparallel}; \frac{\boldsymbol{x}_{\shortparallel}}{\varepsilon}, \frac{x_d}{\varepsilon}\right) \quad \text{in } D^\omega_{\varepsilon H}. \end{aligned}$$

The so-called far-field terms $u^{\omega,FF}_n$ depend only on the macroscopic variable $\boldsymbol{x} := (\boldsymbol{x}_{\shortparallel}, x_d)$ and the so-called near-field terms $U^{\omega,NF}_n$ depend on the tangential components $\boldsymbol{x}_{\shortparallel}$ of $\boldsymbol{x}$ and on the microscopic variable $\boldsymbol{y} := x/\varepsilon$.

We impose that, $\forall n \in \mathbb{N}$, $U^{\omega,NF}_n$ verifies for all $\boldsymbol{x}_{\shortparallel} \in \mathbb{R}^{d-1}$

- $\forall \boldsymbol{y}_{\shortparallel} \in \mathbb{R}^{d-1}$, $\lim_{y_d\to+\infty} U^{\omega,NF}_n(\boldsymbol{x}_{\shortparallel}; \boldsymbol{y}_{\shortparallel}, y_d) = 0$ a.s.,
- $\forall y_d \in \mathbb{R}^+$, $(\omega, \boldsymbol{y}_{\shortparallel}) \mapsto U^{\omega,NF}_n(\boldsymbol{x}_{\shortparallel}; \boldsymbol{y}_{\shortparallel}, y_d)$ stationary.

After injecting the development into the equations verified by u^ω_ε, we obtain for all $n \in \mathbb{N}$

- $u^{\omega,FF}_n$ verifies :

$$\forall \boldsymbol{x} \in D_{\varepsilon,\infty},\ -\Delta u^{\omega,FF}_n(\boldsymbol{x}) - k^2 u^{\omega,FF}_n(\boldsymbol{x}) = f, \quad (1)$$

and the radiation condition.

- $U^{\omega,NF}_n$ satisfies a Laplace-type problem parametrized by $\boldsymbol{x}_{\shortparallel}$ and set in an infinite half-space with a Robin bc on Σ_0 and either a Dirichlet or Neumann bc on $\partial\mathcal{P}^\omega_\varepsilon$. This problem depends on $U^{\omega,NF}_{n-1}$, $U^{\omega,NF}_{n-2}$ and the far-field terms $u^{\omega,FF}_n$ and $u^{\omega,FF}_{n-1}$.

We still need to determine a boundary condition for $u^{\omega,FF}_n$ on $\Sigma_{\varepsilon H}$. This condition will arise as a necessary condition for the existence and uniqueness of the near-field terms.

3 Dirichlet boundary condition on $\partial\mathcal{P}^\omega_\varepsilon$

Let $D^\omega := \mathbb{R}^{d-1}\times(0,H)\backslash\bar{\mathcal{P}}^\omega \bigcup \mathbb{R}^{d-1}\times(H,+\infty)$. In order to study the well-posedness of the problem verified by $U^{\omega,NF}_n$ for $n = 0,1,2$ we consider the following problem : we look for a $\boldsymbol{y}_{\shortparallel}$-stationary solution U^ω to

$$\begin{cases} -\Delta U^\omega & = \nabla\cdot \boldsymbol{G_1}^\omega & \text{in } D^\omega \\ \nabla U^\omega\cdot n & = G_2^\omega & \text{on } \Sigma_0 \\ \quad U^\omega & = 0 & \text{on } \partial\mathcal{P}^\omega \\ \left[\nabla U^\omega\cdot n\right]_H & = G_3^\omega \end{cases} \tag{2}$$

We suppose here that $\boldsymbol{G_1}$, G_2 and G_3 are $\boldsymbol{y}_{\shortparallel}$-stationary processes s.t. $\boldsymbol{G_1}^\omega\in L^2(\Omega,L^2(D^\omega))$, $G_2^\omega\in L^q(\Omega\times\Sigma_0)$, $G_3^\omega\in L^q(\Omega\times\Sigma_H)$, $q\in(2,+\infty]$. We introduce the following space :

$$\mathcal{H}_0 := \Big\{\text{a.s. } U^\omega\in H^1_{loc}(D^\omega)|\ \forall y_d\in\mathbb{R}^+, (\omega,\boldsymbol{y}_{\shortparallel})\mapsto \mathbb{1}_{D^\omega}U^\omega(\boldsymbol{y}_{\shortparallel},y_d) \text{ stationary},\ U^\omega = 0 \text{ on } \partial\mathcal{P}^\omega,\ \mathbb{E}\left[\int_0^{+\infty}\mathbb{1}_{D^\omega}|\nabla U^\omega|^2 dy_d\right] < +\infty\Big\}.$$

Under additional assumptions on $\{x_n\}_{n\in\mathbb{N}^*}$, $\mathcal{H}_0$ can be proven to be a Hilbert space. [2]

Theorem 1 *In this setting, there exists a unique solution U in $\mathcal{H}_0$ to (2). Moreover, there exists $c\in\mathbb{R}$ s.t. a.s. $\lim_{y_d\to+\infty} U^\omega = c$.*

By imposing that a.s. $\lim_{y_d\to+\infty} U^\omega_n = 0$, we get $u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}} = 0$ and $u^{\omega,FF}_1|_{\Sigma_{\varepsilon H}} = c_0^{(1)}\partial_n u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}}$ where $c_0^{(1)}$ is the limit at $+\infty$ of a profile function solution of (2).

4 Neumann boundary condition on $\partial\mathcal{P}^\omega_\varepsilon$

We study the existence and uniqueness of $U^{\omega,NF}_n$ for $n\le 2$. First $\tilde{U}^{\omega,NF}_1 := U^{\omega,NF}_1 - u^{\omega,FF}_1|_{\Sigma_{\varepsilon H}}\chi_{D^\omega_H}$ verifies

$$\begin{cases} -\Delta\tilde{U}^{\omega,NF}_1 & = 0 & \text{in } D^\omega \\ \nabla\tilde{U}^{\omega,NF}_1\cdot n & = -\gamma u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}} & \text{on } \Sigma_0 \\ \nabla\tilde{U}^{\omega,NF}_1.\vec{n} & = -\nabla_{\shortparallel}u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}}\cdot n_{\shortparallel} & \text{on } \partial\mathcal{P}^\omega \\ \left[\nabla\tilde{U}^{\omega,NF}_1\cdot n\right]_H & = \partial_{x_d}u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}} \end{cases} \tag{3}$$

Theorem 2 *If the compatibility condition $-\gamma u^{\omega,FF}_0 + \partial_{x_d}u^{\omega,FF}_0|_{\Sigma_{\varepsilon H}} = 0$ holds, then there exists a unique solution $\tilde{U}^{\omega,NF}_1$ to (3) defined up to a constant in*

$$\mathcal{H} := \Big\{\tilde{U}\in L^2(\Omega,H^1_{loc}(D^\omega))|\ \forall y_3\in\mathbb{R}^+, \mathbb{1}_{D^\cdot}\nabla\tilde{U}^\cdot(\cdot,y_3) \text{ stationary},\ \mathbb{E}\left[\int_0^{+\infty}\mathbb{1}_{D^\omega}|\nabla\tilde{U}^\omega|^2 dy_d\right] < +\infty\Big\}.$$

Given a quantitative mixing assumption on $\{x^\omega_n\}_n$, for d = 3, this solution can be constructed to be $\boldsymbol{y}_{\shortparallel}$-stationary. It then verifies $\lim_{y_d\to\infty}\tilde{U}^{\omega,NF}_1 = 0$.

The proof via regularization relies on classical arguments in stochastic homogenization. [3]

Applying a similar method to $U^{\omega,NF}_2$, the compatibility condition gives us the boundary condition for $u^{\omega,FF}_1$ on $\Sigma_{\varepsilon H}$

$$\nabla u^{\omega,FF}_1.\vec{n} + \gamma u^{FF}_1 = a_0^{(2)}u^{FF}_0 + \sum_{i=1,2} a^{(2)}_{1,i}\partial_{x_i}u^{FF}_0 + a^{(2)}_{2,i}\partial^2_{x_i}u^{FF}_0.$$

The constants $a^{(2)}$ are computed via profile functions solution of type (3) problems.

5 Effective model and error estimates

$v_{2,\varepsilon} :\approx u^{\omega,FF}_0 + \varepsilon u^{\omega,FF}_1$ verifies (1), the radiation condition and on $\Sigma_{\varepsilon H}$

$$(D)\ -\varepsilon c_0^{(1)}\nabla v_{2,\varepsilon}.\vec{n} + v_{2,\varepsilon} = 0,$$

$$(N)\ \nabla v_{2,\varepsilon}.\vec{n} + \left(\gamma - \varepsilon a_0^{(2)}\right)v_{2,\varepsilon} - \varepsilon\sum_{i=1,2} a_i^{(2)}\partial_{x_i}v_{2,\varepsilon} + a_i^{(2)}\partial^2_{x_i}v_{2,\varepsilon} = 0.$$

Theorem 3 (Error estimates for Dirichlet) *For all $M,R>0$,*

$$\sup_{R>0}\mathbb{E}\left[\fint_{\square_R}\int_H^{H+M}|u^\omega_\varepsilon - v_{2,\varepsilon}|^2\,dx\right]^{\frac{1}{2}} = o(\varepsilon).$$

Error estimates in the Neumann case are still in progress.

References

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