

Forward and inverse homogenization of the electromagnetic properties of a quasiperiodic composite

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Abstract

The paper deals with forward and inverse homogenization of Maxwell's equations with a geometry on a microscopic scale given by a quasiperiodic distribution of piecewise constant components defined by the use of a mapping $\mathbf{R} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $m > n$, and a periodic unit cell in \mathbb{R}^m . Inverse homogenization makes use of a Stieltjes analytic representation for the effective complex permittivity, which depends upon \mathbf{R} , unlike for the periodic case.

1 Introduction

The standard setting in homogenization problems for electromagnetic wave propagation is to study periodic material properties in the long wavelength/quasistatic regime. In this paper we consider a heterogeneous material that is periodic in a dimension higher than three, and we use the discovery by Shechtman [12] that quasicrystals can be modeled by taking the cut-and-projection of a periodic structure from a higher dimensional space (typically \mathbb{R}^6 or \mathbb{R}^{12}) onto a hyperplane (such as the Euclidean space \mathbb{R}^3). This problem was mathematically formulated in [8] thanks to a mapping \mathbf{R} from physical space \mathbb{R}^n to higher dimensional space \mathbb{R}^m . This procedure makes it possible to homogenize a class of quasiperiodic materials of physical interest. We refer to [1, 13, 2] for earlier work on this topic. As noted in [1, 13], the homogenized result does not depend upon $\mathbf{R} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, provided it fulfills the criterion

$$\mathbf{R}^T k \neq \mathbf{0}, \forall k \in \mathbb{Z}^m \setminus \{\mathbf{0}\} \quad (1.1)$$

which corresponds to an irrational slope in the one-dimensional case (e.g., $\mathbf{R}^T = (1, \alpha)$, $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ satisfies (1.1)). Some (but not necessarily all) entries of \mathbf{R} are irrational, as a minimum requirement. We call such projections *irrational*, as in [9]. For example, the permittivity of the quasi-crystal Al_{63.5}Fe_{12.5}Cu₂₄ is given by $\mathbf{R} : \mathbb{R}^3 \rightarrow \mathbb{R}^6$,

$$\begin{aligned} \boldsymbol{\varepsilon}(\mathbf{R}x) = & \boldsymbol{\varepsilon}(n_\tau(x_1 + \tau x_2), n_\tau(\tau x_1 + x_3), n_\tau(x_2 + \tau x_3), \\ & n_\tau(-x_1 + \tau x_2), n_\tau(\tau x_1 - x_3), n_\tau(-x_2 + \tau x_3)) \end{aligned}$$

where n_τ is the normalization constant $1/\sqrt{2(2+\tau)}$, with τ the Golden number and $\boldsymbol{\varepsilon} \in L_\sharp^\infty(Y^6)$, i.e., it is periodic and



Figure 1. Composites at different scales.

bounded almost everywhere on the hypercube $Y^6 = [0, 1]^6$.

2 Definition of cut-and-projection partial differential operators

To carry out the analysis of partial differential equations (PDEs) defined on quasiperiodic domains, we need to define differential operators acting in the higher dimensional space \mathbb{R}^m . We let $u \in L^2(Y^m)$, and assume that u is regular enough to make sense to define the cut-and-projected function, $u_{\mathbf{R}} \in L^2(\Omega)$ as $u_{\mathbf{R}}(x) = u(\mathbf{R}x)$. The mapping $y = \mathbf{R}x$ and the chain rule yield the gradient of $u_{\mathbf{R}}$ given by $\nabla u_{\mathbf{R}}(x) = \mathbf{R}^T \nabla_y u(\mathbf{R}x)$. We define \mathbf{R} -dependent differential operators acting on functions defined on domains in \mathbb{R}^m

$$\begin{aligned} \text{grad}_{\mathbf{R}} u(y) &= \mathbf{R}^T \nabla_y u(y) \\ \text{div}_{\mathbf{R}} u(y) &= (\mathbf{R}^T \nabla_y) \cdot u(y) \\ \text{curl}_{\mathbf{R}} u(y) &= (\mathbf{R}^T \nabla_y) \times u(y) \end{aligned}$$

Decompose $W_\sharp^{1,2}(Y^m)$ into two orthogonal spaces,

$$W_\sharp^{1,2}(Y^m) = X \oplus X^\perp,$$

where

$$X = \left\{ u \in W_\sharp^{1,2}(Y^m) \mid \mathbf{R} \mathbf{R}^T \nabla_y u = 0 \right\}$$

and

$$X^\perp = \left\{ u \in W_\sharp^{1,2}(Y^m) \mid (\mathbf{I}_m - \mathbf{R} \mathbf{R}^T) \nabla_y u = 0 \right\} \quad (2.1)$$

with \mathbf{I}_m the identity matrix in \mathbb{R}^m . The space $W^{-1,2}(Y^m)$ can be decomposed of the direct sum of X^- and X^{\perp} which denotes the dual spaces of X and X^\perp . The \mathbf{R} -projected Laplace operator defines a Poisson equation projected on a hyperplane in higher dimension

$$-\Delta_{\mathbf{R}} \theta = f, \quad f \in X^{\perp} \quad (2.2)$$

where $\theta \in X^\perp$ and the \mathbf{R} -projected Laplace-operator is given by $\Delta_{\mathbf{R}} := \nabla_{\mathbf{R}} \cdot \nabla_{\mathbf{R}} = \operatorname{div}_{\mathbf{R}} \mathbf{R} \mathbf{R}^T \operatorname{grad}_{\mathbf{R}}$. Excluding all potentials with gradient components in $\operatorname{Ker} \mathbf{R} \mathbf{R}^T$, which is the same as looking for a solution in X^\perp , makes the problem well posed. Equation (2.2) corresponds to solving Poisson's equation in the projected hyperplane, as in [4, 10].

2.1 Two-scale cut-projection convergence

We define the following function spaces.

$$\mathcal{H}_{\sharp}(\operatorname{div}_{\mathbf{R}}, Y^m) := \left\{ u \in L_{\sharp}^2(Y^m; \mathbb{R}^n) \mid \operatorname{div}_{\mathbf{R}} u \in L_{\sharp}^2(Y^m) \right\}$$

$$\mathcal{H}_{\sharp}(\operatorname{curl}_{\mathbf{R}}, Y^m) := \left\{ u \in L_{\sharp}^2(Y^m; \mathbb{R}^3) \mid \operatorname{curl}_{\mathbf{R}} u \in L_{\sharp}^2(Y^m; \mathbb{R}^3) \right\}$$

$$H(\operatorname{div}, \Omega) := \left\{ u \in L^2(\Omega; \mathbb{R}^n) \mid \operatorname{div} u \in L^2(\Omega) \right\}$$

$$H(\operatorname{curl}, \Omega) := \left\{ u \in L^2(\Omega; \mathbb{R}^3) \mid \operatorname{curl} u \in L^2(\Omega; \mathbb{R}^3) \right\}$$

Definition 2.1 (Weak two-scale convergence). Let Ω be an open bounded set in \mathbb{R}^n and $Y^m =]0, 1[^m$. We say that the sequence (u_η) two-scale converges weakly towards the function $u_0 \in L^2(\Omega \times Y^m)$ for a matrix \mathbf{R} if for every $\varphi \in L^2(\Omega, C_{\sharp}(Y^m))$

$$\lim_{\eta \rightarrow 0} \int_{\Omega} u_\eta(x) \varphi \left(x, \frac{\mathbf{R}x}{\eta} \right) dx = \iint_{\Omega \times Y^m} u_0(x, y) \varphi(x, y) dy \quad (2.3)$$

We denote weak two-scale convergence for a matrix \mathbf{R} with $u_{\eta_k} \xrightarrow{\mathbf{R}} u_0$. The following result [1] ensures the existence of such two-scale limits when the sequence (u_η) is bounded in $L^2(\Omega)$ and \mathbf{R} satisfies (1.1).

Proposition 2.1. Let Ω be an open bounded set in \mathbb{R}^n and $Y^m =]0, 1[^m$. If $\mathbf{R} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is a linear map satisfying (1.1) and (u_η) is a bounded sequence in $L^2(\Omega)$, then there exist a vanishing subsequence η_k and a limit $u_0(x, y) \in L^2(\Omega \times Y^m)$ (Y^m -periodic in y) such that $u_{\eta_k} \xrightarrow{\mathbf{R}} u_0$ as $\eta_k \rightarrow 0$.

Proposition 2.2. Let $\{u_\eta\}$ be a uniformly bounded sequence in $H(\operatorname{curl}, \Omega)$. Then there exist a subsequence $\{u_{\eta_k}\}$ and functions $u_0 \in H(\operatorname{curl}, \Omega, \mathcal{H}_{\sharp}(\operatorname{curl}_{\mathbf{R}_0}, Y^m))$, $\operatorname{grad}_{\mathbf{R}} \phi \in L^2(\Omega, L_{\sharp}^2(Y^m; \mathbb{R}^3))$, and $\operatorname{curl}_{\mathbf{R}} u_1 \in L^2(\Omega, L_{\sharp}^2(Y^m; \mathbb{R}^3))$ such that

$$u_{\eta_k} \xrightarrow{\mathbf{R}} u_0(x, y) = u(x) + \operatorname{grad}_{\mathbf{R}} \phi(x, y) \quad (2.4)$$

$$\operatorname{curl} u_{\eta_k} \xrightarrow{\mathbf{R}} \operatorname{curl} u(x) + \operatorname{curl}_{\mathbf{R}} u_1(x, y) \quad (2.5)$$

as $\eta_k \rightarrow 0$, where

$$u(x) = \int_{Y^m} u_0(x, y) dy$$

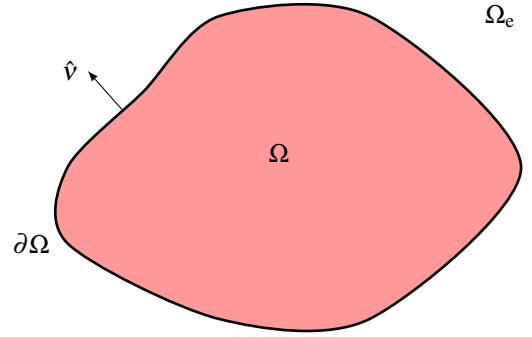


Figure 2. Typical geometry of the scattering problem. The domain Ω , its boundary $\partial\Omega$, the unit normal vector \hat{v} and the exterior Ω_e .

Proposition 2.3. Let $\{u_\eta\}$ be a uniformly bounded sequence in $H(\operatorname{div}, \Omega)$. Then there exist a subsequence $\{u_{\eta_k}\}$ and functions $u_0 \in H(\operatorname{div}, \Omega, \mathcal{H}_{\sharp}(\operatorname{div}_{\mathbf{R}_0}, Y^m))$ and $\operatorname{div}_{\mathbf{R}} u_1 \in L^2(\Omega, L_{\sharp}^2(Y^m))$ such that

$$u_{\eta_k} \xrightarrow{\mathbf{R}} u_0(x, y) \quad (2.6)$$

$$\operatorname{div} u_{\eta_k} \xrightarrow{\mathbf{R}} \operatorname{div} u(x) + \operatorname{div}_{\mathbf{R}} u_1(x, y) \quad (2.7)$$

as $\eta_k \rightarrow 0$, where

$$u(x) = \int_{Y^m} u_0(x, y) dy$$

2.2 The heterogeneous Maxwell's equations

Let Ω be an open, bounded domain in \mathbb{R}^3 with simply connected Lipschitz boundary $\partial\Omega$. We denote the exterior of the domain Ω by $\Omega_e = \mathbb{R}^3 \setminus \overline{\Omega}$, which is assumed to be simply connected.

The scattered electromagnetic field satisfies the exterior problem outside the scattering domain

$$\begin{cases} \nabla \times E_s(x) = ik_0 H_s(x), \\ \nabla \times H_s(x) = -ik_0 E_s(x), \end{cases} \quad x \in \Omega_e. \quad (2.8)$$

where k_0 is the wavenumber in vacuum. The scattered fields satisfy the Silver–Müller radiation condition at infinity, i.e., one of the following conditions (see [7]):

$$\begin{cases} \hat{v} \times E_s(x) - H_s(x) = o(1/|x|), \\ \hat{v} \times H_s(x) + E_s(x) = o(1/|x|) \end{cases} \quad \text{as } |x| \rightarrow \infty \quad (2.9)$$

uniformly in all directions.

In Ω_e the sum of the incident and the scattered fields is defined as the total field, i.e.,

$$\begin{cases} E_t(x) = E_i(x) + E_s(x), \\ H_t(x) = H_i(x) + H_s(x), \end{cases} \quad x \in \Omega_e.$$

The boundary conditions on $\partial\Omega$ are

$$\begin{cases} \hat{\mathbf{v}} \times E_i|_{\partial\Omega} + \hat{\mathbf{v}} \times E_s|_{\partial\Omega} = \hat{\mathbf{v}} \times E|_{\partial\Omega}, \\ \hat{\mathbf{v}} \times H_i|_{\partial\Omega} + \hat{\mathbf{v}} \times H_s|_{\partial\Omega} = \hat{\mathbf{v}} \times H|_{\partial\Omega}, \end{cases} \quad (2.10)$$

where E and H solve an interior problem (in Ω). The system (2.8) with the radiation condition (2.9) supplied with the boundary condition

$$\hat{\mathbf{v}} \times E_s|_{\partial\Omega} = m \in H^{-\frac{1}{2}}(\text{div}, \partial\Omega),$$

has a unique solution $(E_s, H_s) \in H_{\text{loc}}(\text{curl}, \overline{\Omega}_e) \times H_{\text{loc}}(\text{curl}, \overline{\Omega}_e)$ for any $m \in H^{-\frac{1}{2}}(\text{div}, \partial\Omega)$ [3, p. 107].

The permittivity and permeability are assumed to be coercive and bounded. The interior problem for a heterogeneous material contained in the domain Ω reads

$$\begin{cases} \nabla \times E^\eta(x) = ik_0 B^\eta(x), \\ \nabla \times H^\eta(x) = -ik_0 D^\eta(x), \end{cases} \quad x \in \Omega,$$

almost everywhere, with boundary conditions given by (2.10). By using the constitutive relations for the higher dimensional periodic material,

$$\begin{cases} D^\eta(x) = \varepsilon(\frac{\mathbf{R}_x}{\eta}) \cdot E^\eta(x), \\ B^\eta(x) = \mu(\frac{\mathbf{R}_x}{\eta}) \cdot H^\eta(x), \end{cases} \quad x \in \Omega,$$

we eliminate D^η, B^η and obtain the quasiperiodic formulation of the Maxwell's equations

$$\begin{cases} \nabla \times E^\eta(x) = ik_0 \mu(\frac{\mathbf{R}_x}{\eta}) \cdot H^\eta(x), \\ \nabla \times H^\eta(x) = -ik_0 \varepsilon(\frac{\mathbf{R}_x}{\eta}) \cdot E^\eta(x) \end{cases} \quad x \in \Omega, \quad (2.11)$$

where the solution (E^η, H^η) is in $H(\text{curl}, \Omega) \times H(\text{curl}, \Omega)$. In the homogenization procedure we identify the limit of the fields E^η, H^η when $\eta \rightarrow 0$. This limit satisfies the homogenized system with constant coefficients, which is a model of a homogeneous material. We have the uniform a priori estimate

$$\|E^\eta\|_{H(\text{curl}, \Omega)} + \|H^\eta\|_{H(\text{curl}, \Omega)} \leq C,$$

2.3 The homogenized Maxwell's equations

The homogenized Maxwell's equations for periodic composites is given in [14] and read

$$\begin{cases} \nabla \times E(x) = ik_0 \mu^h \cdot H(x), \\ \nabla \times H(x) = -ik_0 \varepsilon^h \cdot E(x) \end{cases} \quad (2.12)$$

where E and H belongs to $H(\text{curl}, \Omega)$. The system is coupled to the exterior problem (2.8) via the boundary conditions (2.10). The homogenized permeability and permittivity ε^h and μ^h are defined by

$$\varepsilon_{ik}^h = \int_{Y^m} \varepsilon_{ij}(y) \left(\delta_{jk} - \nabla_{y_j} \chi_e^k(y) \right) dy$$

$$\mu_{ik}^h = \int_{Y^m} \mu_{ij}(y) \left(\delta_{jk} - \nabla_{y_j} \chi_h^k(y) \right) dy$$

where the potentials χ_e^k and χ_h^k solve the local equations

$$\int_{Y^m} \varepsilon_{ij}(y) \left(\delta_{jk} - \nabla_{y_j} \chi_e^k(y) \right) \nabla_{y_i} \phi(y) dy = 0 \quad (2.13)$$

$$\int_{Y^m} \mu_{ij}(y) \left(\delta_{jk} - \nabla_{y_j} \chi_h^k(y) \right) \nabla_{y_i} \phi(y) dy = 0 \quad (2.14)$$

Propositions 2.1, 2.2, and 2.3 yields the quasiperiodic case of the homogenized material properties

$$\varepsilon_{ik}^h = \int_{Y^m} \varepsilon_{ij}(y) \left(\delta_{jk} - (\mathbf{R}_j^T \nabla_y) \chi_e^k(y) \right) dy$$

$$\mu_{ik}^h = \int_{Y^m} \mu_{ij}(y) \left(\delta_{jk} - (\mathbf{R}_j^T \nabla_y) \chi_h^k(y) \right) dy$$

where the projected gradients $(\mathbf{R}_j^T \nabla_y) \chi_e^k$ and $(\mathbf{R}_j^T \nabla_y) \chi_h^k$ solve the local equations

$$\int_{Y^m} \varepsilon_{ij}(y) \left(\delta_{jk} - (\mathbf{R}_j^T \nabla_y) \chi_e^k(y) \right) (\mathbf{R}_i^T \nabla_y) \phi(y) dy = 0 \quad (2.15)$$

$$\int_{Y^m} \mu_{ij}(y) \left(\delta_{jk} - (\mathbf{R}_j^T \nabla_y) \chi_h^k(y) \right) (\mathbf{R}_i^T \nabla_y) \phi(y) dy = 0 \quad (2.16)$$

3 Stieltjes analytic representation for the effective conductivity

From now on we assume that the electric permittivity is piecewise constant on the unit cell in \mathbb{R}^m , i.e.,

$$\varepsilon(y) = \varepsilon_1 \chi_1(y) + \varepsilon_2 \chi_2(y) = \varepsilon_1 \chi_1(y) + (1 - \chi_1(y)) \varepsilon_2, \quad (3.1)$$

where ε_1 and ε_2 are coercive (complex) and scalar valued bounded constants, χ_1 and χ_2 are the characteristic functions of medium 1 and 2, respectively. They are periodic in \mathbb{R}^m , hence the scaled (and projected) permittivity function, $\varepsilon(\frac{\mathbf{R}_x}{\eta})$, is quasiperiodic in \mathbb{R}^n . A similar assumption is assumed for the permeability, μ . The local equation (2.15) in a strong formulation reads

$$-\text{div}_y \mathbf{R} \varepsilon(y) \mathbf{R}^T \text{grad}_y \chi_e^k(y) = -\text{div}_y \mathbf{R} \varepsilon(y) e_k$$

The material distribution in the unit cell as given in (3.1) and some algebra yields

$$(s \mathbf{I}_n - \Gamma_{\mathbf{R}} \chi_1(y)) (e_k - \nabla_{\mathbf{R}} \chi_e^k(y)) = s e_k$$

where $s = \varepsilon_2 / (\varepsilon_2 - \varepsilon_1)$ and $\Gamma_{\mathbf{R}} := \nabla_{\mathbf{R}} (\Delta_{\mathbf{R}})^{-1} \nabla_{\mathbf{R}}$. Applying the inverse of the operator on the left hand side yields

$$e_k - \nabla_{\mathbf{R}} \chi_e^k(y) = s (s \mathbf{I}_n - \Gamma_{\mathbf{R}} \chi_1(y))^{-1} e_k$$

The spectral resolution of $\Gamma_{\mathbf{R}} \chi_1$ with the \mathbf{R} -projected projection valued measure $Q_{\mathbf{R}}$ gives [11]

$$E^k(s) = e_k - \nabla_{\mathbf{R}} \chi_e^k(y) = \int_0^1 \frac{s}{s-z} dQ_{\mathbf{R}}(z) e_k \quad (3.2)$$

We define a function F_{kl} which measures how the homogenized property of the composite depends on the contrast between the components

$$F_{kl}(s) = 1 - \frac{\varepsilon_{kl}^h}{\varepsilon_2} = 1 - \frac{\langle \varepsilon E^k, e_l \rangle}{\varepsilon_2} = \langle s^{-1} \chi_1 E^k, e_l \rangle$$

The integral representation of this function is obtained using (3.2) as

$$F_{kl}(s) = \langle \chi_1(y) (s \mathbf{I}_n - \Gamma_{\mathbf{R}} \chi_1(y))^{-1} e_k, e_l \rangle = \int_0^1 \frac{\langle \chi_1 dQ_{\mathbf{R}}(z) e_k, e_l \rangle}{s - z}$$

Let \mathcal{M}_{kl} be a positive tensor measure corresponding to the spectral measure $Q_{\mathbf{R}}$, so that $d\mathcal{M}_{kl}(z) = \langle \chi_1 dQ_{\mathbf{R}}(z) e_k, e_l \rangle$, then

$$F_{kl}(s) = \int_0^1 \frac{d\mathcal{M}_{kl}(z)}{s - z}$$

This representation separates information about the microstructure of the composite material, which is contained in the spectral measure \mathcal{M} from information about the properties of the materials. It was shown in [6, 5] that in the case of random or periodic composites, the spectral measure \mathcal{M} in this integral representation can be uniquely reconstructed from values of the function F available on an arc in the complex plane. Here we extend the result to the quasiperiodic case.

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