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Quasiperiodic Composites: Multiscale Reiterated Homogenization

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Abstract – **With recent technological advances, quasiperiodic and aperiodic materials present a novel class of metamaterials that possess very unusual, extraordinary properties such as superconductivity, unusual mechanical properties and diffraction patterns, extremely low thermal conductivity, etc. As all these properties critically depend on the microgeometry of the media, the methods that allow characterizing the effective properties of such materials are of paramount importance. In this paper, we analyze the effective properties of a class of multiscale composites consisting of periodic and quasiperiodic phases appearing at different scales. We derive homogenized equations for the effective behavior of the composite and discover a variety of new effects which could have interesting applications in the control of wave and diffusion phenomena.**

I. Introduction

Discovery of a quasicrystalline material by Shechtman [5], exhibiting unusual ten-fold electron diffraction pattern, has overturned our notion of crystallographic symmetries and led to a completely new class of materials with very unusual properties and with the microstructures possessing a long-range order and lacking translational symmetry. Though the first quasicrystalline materials were thermodynamically unstable, since their discovery, many stable materials were found and efficient technologies able to produce them, were developed [4]. Mathematically, quasicrystals can be modeled by cutting and projecting a periodic structure from a higher dimensional space (typically $\mathbb{R}^6$ or $\mathbb{R}^{12}$) onto a hyperplane (such as the Euclidean space $\mathbb{R}^3$), that was formulated in [3] using a mapping $\mathbf{R}$ from physical space $\mathbb{R}^n$ to upper dimensional space $\mathbb{R}^m$. This cut-and-projection procedure allows to homogenize quasiperiodic materials of physical interest [2, 6]. As noted in [2, 6], the homogenized result does not depend upon $\mathbf{R} : \mathbb{R}^n \to \mathbb{R}^m$, provided it fulfills the criterion

$$\mathbf{R}^T \boldsymbol{k} \neq \mathbf{0} \ , \ \forall \boldsymbol{k} \in \mathbb{Z}^m \setminus \{\mathbf{0}\} \tag{1}$$

This criterion corresponds to an irrational slope in the one-dimensional case (e.g. $\mathbf{R}^T = (1, \alpha)$ where α is irrational, satisfies (1), see Fig. 1 where the slope $\alpha = \tan\phi$). As an example, the conductivity of the quasicrystal $Al_{63.5}Fe_{12.5}Cu_{24}$ is given by $\mathbf{R} : \mathbb{R}^3 \to \mathbb{R}^6$,

$$\begin{aligned}\sigma\big(\mathbf{R}\boldsymbol{x}\big) = \ & \sigma\big(n_\tau(x_1 + \tau x_2), n_\tau(\tau x_1 + x_3), n_\tau(x_2 + \tau x_3),\\ & n_\tau(-x_1 + \tau x_2), n_\tau(\tau x_1 - x_3), n_\tau(-x_2 + \tau x_3)\big)\end{aligned} \tag{2}$$

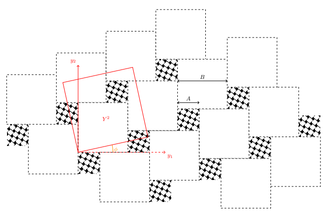

Fig. 1: Multiscale homogenization: cut-and-projection slope $\alpha = \tan\phi$

where n_τ is the normalization constant $1/\sqrt{2(2+\tau)}$ with the Golden number τ and $\sigma \in \mathrm{L}^\infty_\#(Y^6)$, i.e. it is periodic and bounded almost everywhere on the hypercube $Y^6 =]0,1[^6$. Here we extend the cut-and-projection method to multiscale reiterated homogenization, see Fig.1.

Let Ω denote a bounded open set in $\mathbb{R}^n$. Let us recall the definition of the cut-and-project two-scale convergence as introduced by Bouchitté and co-authors in 2010 [2].

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Definition I..1 *Given a matrix* $\mathbf{R} \in \mathcal{M}^{m\times n}$ *satisfying the condition* (1)*, a family* $u_\eta(x)$ *in* $\mathrm{L}^2(\Omega)$ *is said to two-scale cut-and-project converge to a multiscale limit* $u_0(x,y) \in \mathrm{L}^2(\Omega \times Y^m)$ *if the following limit holds*

$$\lim_{\eta\to 0} \int_\Omega u_\eta(x)\psi\left(x, \frac{\mathbf{R}x}{\eta}\right) \mathrm{d}x = \int_\Omega \int_{Y^m} u_0(x,y)\psi(x,y)\,\mathrm{d}y\,\mathrm{d}x$$

for all $\psi(x,y) \in \mathrm{L}^2(\Omega; \mathrm{C}_\#(Y^m))$.

The two scale cut-and-project method makes it possible to homogenize a class of quasiperiodic materials [2, 6], for which one cannot easily define a concept of long wavelength limit (due to the fact that quasiperiods can be arbitrarily large). Here we are extending the method to multiscale quasiperiodic composites. In particular, we are interested in finding answers to the following questions:

- Is it possible to extend the theory to handle both *periodic* and *quasiperiodic* oscillations of the structure at the same scale?
- Is it possible to extend the theory to handle *quasiperiodic* oscillations at multiple scales?

II. Reiterated Convergence and Homogenization

To address these questions, we consider reiterated convergence following the approach developed by Allaire and Briane [1]. We consider here the case when the scales of microstructural oscillations are well separated and introduce multiscale cut-and-project convergence.

Definition II..1 *Let* $\Omega \subset \mathbb{R}^d$ *be a bounded open set and let* $Y^m := [0,1)^m$ *denote the* m*-dimensional unit cubes for any* $m \in \mathbb{N}$*. Given the matrices* $\mathbf{R}_i \in \mathcal{M}^{m_i \times d}$ *satisfying the condition* (1) *for each* $i \in \{1,\dots,N\}$ *with* $m_i \in \mathbb{N}$ *and* $m_i \geq d$*. A family* $u_\eta(x)$ *in* $\mathrm{L}^2(\Omega)$ *is said to multiscale cut-and-project converge to a limit* $u_0(x, y_1, \dots, y_N) \in \mathrm{L}^2(\Omega \times Y^{m_1} \times \cdots Y^{m_N})$ *if the following limit holds*

$$\lim_{\eta\to 0} \int_\Omega u_\eta(x)\psi\left(x, \frac{\mathbf{R}_1 x}{\eta_1}, \dots, \frac{\mathbf{R}_N x}{\eta_N}\right) \mathrm{d}x$$
$$= \int_\Omega \int_{Y^{m_1}} \cdots \int_{Y^{m_N}} u_0(x, y_1, \dots, y_N)\psi(x, y_1, \dots, y_N)\,\mathrm{d}y_N \cdots \,\mathrm{d}y_1\,\mathrm{d}x$$

for all $\psi(x, y_1, \dots, y_N) \in \mathrm{L}^2(\Omega; \mathrm{C}_\#(Y^{m_1}) \times \cdots \times \mathrm{C}_\#(Y^{m_N}))$.

Now we can formulate our main theorem.

Theorem II..1 *Let* $u_\eta(x)$ *be a uniformly bounded family in* $\mathrm{H}^1(\Omega)$*, i.e.*

$$\|u_\eta\|_{\mathrm{H}^1(\Omega)} \leq C$$

with C *being independent of* η*. Then, up to extraction of subsequence, we have*

$$u_\eta \rightharpoonup u_0(x, y_1, \dots, y_N) \tag{3}$$

$$\nabla u_\eta \rightharpoonup \nabla_x u_0(x, y_1, \dots, y_N) + \sum_{i=1}^{N} \mathbf{R}_i^\top \nabla_{y_i} u_i(x, y_1, \dots, y_i) \tag{4}$$

in the sense of multiscale cut-project convergence (see Definition II..1*). Furthermore*

$$\mathbf{R}_i^\top \nabla_{y_i} u_0(x, y_1, \dots, y_N) = 0 \qquad \forall i \in \{1, \dots, N\}. \tag{5}$$

Consider the following multiscale boundary value problem with quasiperiodic microstructure described by the matrices $\mathbf{R}_1, \cdots, \mathbf{R}_N$ corresponding to different scales $\eta_1, \cdots, \eta_N$:

$$\begin{cases} -\mathrm{div}\left(A\left(x, \dfrac{\mathbf{R}_1 x}{\eta_1}, \cdots, \dfrac{\mathbf{R}_N x}{\eta_N}\right)\nabla u_\eta(x)\right) = f(x) & \text{in } \Omega, \\ u_\eta(x) = 0 & \text{on } \partial\Omega. \end{cases} \tag{6}$$

Dictated by the multiscale limits, we test the above equation by the test functions

$$\varphi_0\left(x, \frac{\mathbf{R}_1 x}{\eta_1}, \cdots, \frac{\mathbf{R}_N x}{\eta_N}\right) + \sum_{k=1}^{N} \eta_k\, \varphi_k\left(x, \frac{\mathbf{R}_1 x}{\eta_1}, \cdots, \frac{\mathbf{R}_N x}{\eta_N}\right) \tag{7}$$

where the φ_k's satisfy for each $k \in \{0, 1, \dots. N-1\}$,

$$\mathbf{R}_{k+j}^{\top} \nabla_{y_{k+j}} \varphi_k = 0 \qquad \forall j = 1, \dots, N-k. \tag{8}$$

Passing to the limit in the weak formulation of the problem results in the variational formulation of the following $N+1$-scale homogenized problem:

$$\begin{cases} -\mathrm{div}_{y_N}\left(\mathbf{R}_N A\left(\nabla_x u_0 + \sum_{k=1}^{N} \mathbf{R}_k^{\top} \nabla_{y_k} u_k\right)\right) = 0, \\ -\mathrm{div}_{y_j}\left(\int_{Y^{m_{j+1}}} \cdots \int_{Y^{m_N}} \mathbf{R}_j A\left(\nabla_x u_0 + \sum_{k=1}^{N} \mathbf{R}_k^{\top} \nabla_{y_k} u_k\right) \prod_{l=j+1}^{N} \mathrm{d}y_l\right) = 0 \quad \text{for } 1 \le j \le N-1, \\ -\mathrm{div}_x\left(\int_{Y^{m_1}} \cdots \int_{Y^{m_N}} A\left(\nabla_x u_0 + \sum_{k=1}^{N} \mathbf{R}_k^{\top} \nabla_{y_k} u_k\right) \prod_{l=1}^{N} \mathrm{d}y_l\right) = f(x) \end{cases} \tag{9}$$

This result shows that the homogenized effective property is obtained by reiteration of n quasiperiodic (in the sense of cut-and-projection) homogenization problems, successively from the smallest to the largest scale.

III. Conclusion

Based on two-scale reiterated convergence and the cut-and-projection method, we have developed an approach to the homogenization of multiscale periodic and quasiperiodic media or different quasiperiodic media mixed on different scales. We have shown that the effective property and homogenized fields can be obtained by iteratively solving a sequence of homogenization problems. This is the first theoretical result on homogenization of multiscale quasiperiodic materials that lays the foundation for further theoretical developments and numerical methods for a novel class of composites that could be termed as 'multiscale irrational metamaterials'.

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