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Multiple scale method applied to homogenization of irrational metamaterials

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Abstract – **We adapt the multiple scale method introduced over 40 years ago for the homogenization of periodic structures [1], to the quasiperiodic (cut-and-projection) setting. We make use of partial differential operators (gradient, divergence and curl) acting on periodic functions of m variables in a higher-dimensional space that are projected onto operators acting on quasiperiodic functions in the n-dimensional physical space ($m > n$). We replace heterogeneous quasiperiodic structures, coined irrational metamaterials in [2], by homogeneous media with anisotropic permittivity and permeability tensors, obtained from the solution of annex problems of electrostatic type in a periodic cell in higher dimensional space. This approach is valid when the wavelength is much larger than the period of the higher dimensional elementary cell.**

I. Introduction

It was numerically shown over twenty years ago that photonic quasicrystals (PQs) have very peculiar diffraction properties: In complete contradiction with the periodic or random cases, PQs exhibit forbidden bands (i.e. perfect reflection) at extremely large wavelengths [3]. This can be attributed to the fact that there is always a quasiperiod in resonance with the wavelength, no matter how large it is, at least in the infinite quasiperiodic case. This Bragg scattering in the long wavelength limit indicates that the homogenization process might be more difficult to perform for PQs than for photonic crystals. It was shown in [4] that dielectric PQs derived from a cut-and-projection of periodic structure in a higher dimensional space [5] can be replaced by an effective anisotropic dielectric medium. However, the homogenized problem was written in an abstract mathematical setting, not very amenable to numerical solution, since the differential operators curl, gradient and divergence, were defined in a Fourier space. This issue was resolved in [6], thanks to the introduction of irrational differential operators defined in well-suited functional spaces. In this article, we briefly recall the cut-and-project method introduced by Duneau and Katz [5], we further discuss the irrational (cut-and-project) differential operators introduced in [6] and then proceed with the asymptotic analysis of the Maxwell's system for quasi-periodic (cut-and-project) PQs structures.

II. The cut-and-project method

Let us note here that PQs derived from a cut-and-projection include important cases such as the metallic phase discovered by Shechtman and coauthors in 1984 [9], as well as PQs engineered in [7, 8]. Three-dimensional PQs can be thought of as the projection of a six-dimensional crystal onto three dimensions. Such 3D PQs possess a long-range order but no periodicity. As a result, the corresponding diffraction diagrams exhibit an infinite number of diffraction peaks in any finite solid angle, in sharp contrast to crystals and random media.

It is hard to visualize a periodic structure in 6D space, so the method is best illustrated with a cut-and-projection of a biperiodic structure in 2D onto a 1D quasiperiodic structure, as shown in Fig. 1, where it should be noted that the slope of the 1D quasiperiodic line is irrational. The cut-and-project quasiperiodic tiling is built from a biperiodic tiling made of identical rectangles tilted at an angle θ. The projection is onto the straight line with a slope $\tan\theta$. We represent the straight line $x_2 = \tan\theta x_1$ in blue and in purple on the periodic cell $Y = [0,1]^2$ with the same number of segments. With the rational slope, the segments would go back to the same place whereas with an irrational slope such as the Golden number $\tau = (1+\sqrt{5})/2$, the segments "scan" the whole unit, enabling to reconstruct the cell : That is one of the secrets of the homogenization method applied here.

The cut-and-project method described above can be viewed as a rotation of axes in 2D periodic space. We would like now to generate an 3D icosahedral PQ, we need a 6D hypercube which has 64 corners, 192 edges, 240 2D faces, 160 3D faces (cells), 60 4D faces (hypercells) and 12 5D faces. It is obviously hard to visualize, so we shall just proceed with algebraic representation of the cut-and-project with the rotation matrix in 6D periodic space.

We can consider for instance the matrix $\mathbf{M}$ which expresses the basis vectors $\mathbf{E}_q$, $q = 1, ..., 6$ in $\mathbb{Z}^6$ in terms of the basis vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ of the projected subspace $E_\parallel$ (the blue line in Fig. 1) and the basis vectors $\mathbf{e}_4$, $\mathbf{e}_5$ and $\mathbf{e}_6$ of the orthogonal subspace $\mathcal{E}_\parallel$: $\mathbf{E}_q = \sum_{l=1}^{6} M_{ql}\mathbf{e}_l$, with

$$\mathbf{M} = \frac{1}{\sqrt{2\tau^2+1}} \begin{pmatrix} \tau & \tau & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & \tau & 1 & \tau \\ 1 & -1 & -\tau & 0 & \tau & 0 \\ \tau & -\tau & 1 & 0 & -1 & 0 \\ -1 & -1 & 0 & -\tau & 0 & \tau \\ 0 & 0 & \tau & -1 & \tau & -1 \end{pmatrix} \tag{1}$$

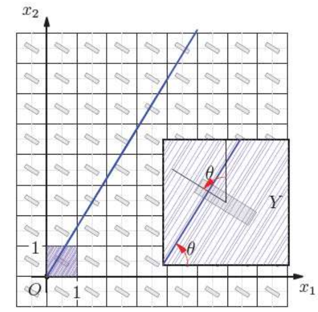

Fig. 1: Cut-and-project method

$\mathbf{M}$ maps a six-dimensional coordinate vector onto another one whose first three components represent the cut-and-projected coordinates in physical space.

Now from $\mathbf{M}$ we construct the matrix $\mathbf{R}$ (resp. $\mathbf{P}$) with its first three rows, which is associated with the mapping from physical space $\mathbb{R}^3$ to higher dimensional space $\mathbb{R}^6$ (resp. from $\mathbb{R}^6$ to $\mathbb{R}^3$). Besides $\mathbf{R}$ is one left pseudo-inverse of $\mathbf{P}$ i.e. $\mathbf{RP} = \mathbf{I}_3$, where $\mathbf{I}_3$ is the identity in $\mathbb{R}^3$. One notes that $\mathbf{R}$ is not unique, which could be an issue in the definition of the effective properties of quasi-crystals. However, both matrices fulfill the criterion

$$\mathbf{P}\boldsymbol{k} \neq \mathbf{0}_3 \text{ and } \mathbf{R}^T\boldsymbol{k} \neq \mathbf{0}_3 \ , \ \forall \boldsymbol{k} \in \mathbb{Z}^6 \setminus \{\mathbf{0}_6\} \ . \tag{2}$$

This criterion means that the entries of $\mathbf{P}$ and $\mathbf{R}$ are incommensurate. This criterion underpins the homogenization theory of PQs, which we have developed as it makes the homogenized problem uniquely defined [4, 6].

III. Asymptotic analysis and main homogenization result

Homogenization of the quasi-periodic Maxwell system using the concept of two-scale-cut-and-project convergence has been performed in [4, 6]. Here, we would like to propose an asymptotic analysis of the quasi-periodic Maxwell system, by adapting two-scale expansion techniques developed in [1] to quasi-periodic structures. Our illustrative example is the Maxwell system, but our approach can be applied to any partial differential equation (PDE) with fast oscillating coefficients of the form $a(\mathbf{R}(\boldsymbol{x})/\eta)$, with $\boldsymbol{x}$ the position vector in physical space $\mathbb{R}^3$, η a small positive parameter and where $a(\boldsymbol{y})$ is a Y-periodic function, with $Y = [0;1]^6$ a periodic cell in upper dimensional space $\mathbb{R}^6$. Asymptotic expansion of fast oscillatory field $\boldsymbol{u}_\eta(\boldsymbol{x})$ solution of the PDE takes the form

$$\boldsymbol{u}_\eta(\boldsymbol{x}) = \boldsymbol{u}_0(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) + \eta\boldsymbol{u}_1(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) + \eta^2\boldsymbol{u}_2(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) + ... \ , \tag{3}$$

where $\boldsymbol{u}_i(\boldsymbol{x}, \boldsymbol{y})$, $i = 0, 1, ...$, are Y-periodic functions in $\boldsymbol{y}$ with enough regularity in $\boldsymbol{x}$ and $\boldsymbol{y}$. We note that the rescaled gradient acting on two-scale functions $\boldsymbol{u}_i$ is such that

$$\nabla\, \boldsymbol{u}_i(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) = \nabla_{\boldsymbol{x}}\, \boldsymbol{u}_i(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) + \eta^{-1}\nabla_{\mathbf{R}}\, \boldsymbol{u}_i(\boldsymbol{x}, \mathbf{R}(\boldsymbol{x})/\eta) \ , \tag{4}$$

where the so-called cut-and-projection operator $\nabla_{\mathbf{R}}\, \boldsymbol{u}_i(\boldsymbol{x}, \boldsymbol{y}) = \mathbf{R}^T\nabla_{\boldsymbol{y}}\, \boldsymbol{u}_i(\boldsymbol{x}, \boldsymbol{y})$. Rescaled divergence and curl have similar expressions. We shall see that one can then carry out asymptotic analysis of the Maxwell system in a way similar to what was done in [11] for the periodic case.

We consider a fixed finite bounded domain $\Omega_f \subset \mathbb{R}^3$, filled with a quasicrystal occupying the domain $\Omega_\eta \subset \Omega_f$, such as shown in Figure 2. When a small positive parameter η goes to zero, the number of spherical scatterers inside the quasi-periodic scaffolding Ω_η tends to infinity while their size tends to zero and in this way Ω_η gets bigger and bigger and tends to Ω_f. Let $\mathbf{H}_\eta$ be a sequence of magnetic fields solutions of the diffraction problems

$$(\mathcal{P}_\eta^{\boldsymbol{H}}) \begin{cases} \nabla\times\varepsilon^{-1}(\boldsymbol{x}, \frac{\mathbf{R}\boldsymbol{x}}{\eta})\nabla\times\boldsymbol{H}_\eta - k_0^2\mu(\boldsymbol{x}, \frac{\mathbf{R}\boldsymbol{x}}{\eta})\boldsymbol{H}_\eta = \mathbf{0} & , \text{ in } \mathbb{R}^3 \\ \boldsymbol{H}_\eta^d = O(\frac{1}{|\boldsymbol{x}|}) & , \text{ in } \mathbb{R}^3 \setminus \bar{\Omega}_\eta \\ \frac{\boldsymbol{x}}{|\boldsymbol{x}|}\times\nabla\times\boldsymbol{H}_\eta^d + ik\boldsymbol{H}_\eta^d = o(\frac{1}{|\boldsymbol{x}|}) & , \text{ in } \mathbb{R}^3 \setminus \bar{\Omega}_\eta \end{cases}$$

where $\boldsymbol{H}_\eta^d$ is the diffracted field deduced from the incident field $\boldsymbol{H}^i$ illuminating the quasicrystal by $\boldsymbol{H}_\eta^d = \boldsymbol{H}_\eta - \boldsymbol{H}^i$, $k_0 = \omega/c$ is the wave number, ω is the angular frequency, c is the speed of light, $\tilde{\varepsilon}(\boldsymbol{x}, \frac{\mathbf{R}\boldsymbol{x}}{\eta})$ and $\tilde{\mu}(\boldsymbol{x}, \frac{\mathbf{R}\boldsymbol{x}}{\eta})$ respectively denote the relative permittivity and permeability of the medium.

As η tends to zero, we would like to replace the heterogeneous diffracting medium of shape Ω_η, by a homogeneous medium of shape Ω_f with both anisotropic permittivity and permeability.

We find that the limit problem is

$$(\mathcal{P}^{\boldsymbol{H}}_{hom}) = \begin{cases} \nabla\times([\varepsilon^{-1}_{hom}](\boldsymbol{x})\nabla\times\boldsymbol{H}_{hom}(\boldsymbol{x})) - k_0^2[\mu_{hom}]\boldsymbol{H}_{hom}(\boldsymbol{x}) = \mathbf{0} \\ \boldsymbol{H}^d_{hom}(\boldsymbol{x}) = O(1|\ \boldsymbol{x}\ |) \\ \frac{\boldsymbol{x}}{|\boldsymbol{x}|}\times\nabla\times\boldsymbol{H}^d_{hom}(\boldsymbol{x}) + ik\boldsymbol{H}^d_{hom}(\boldsymbol{x}) = o(\frac{1}{|\boldsymbol{x}|}) \end{cases}$$

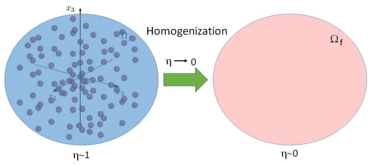

Fig. 2: Homogenization of irrational metamaterial made of identical spherical scatterers.

with

$$\begin{cases} [\varepsilon_{hom}](\boldsymbol{x}) =< \varepsilon(\boldsymbol{x},\boldsymbol{y})(\mathbf{I}_3 - \nabla_{\mathbf{R}}\boldsymbol{V}_Y(\boldsymbol{y})) >_Y & \text{, in } \Omega_f \\ [\varepsilon_{hom}](\boldsymbol{x}) = \mathbf{I}_3 & \text{, in } \Omega_f^c \end{cases} \quad (5)$$

and a similar expression for the homogenized magnetic permeability. Here the so-called cut-and-project operator $\nabla_{\mathbf{R}} = \mathbf{R}^T\nabla_{\boldsymbol{y}}$ and $< f >_Y$ is the average of f in Y (i.e. $\int_Y f(\boldsymbol{x},\boldsymbol{y})\ \mathrm{d}\boldsymbol{y}$). $\boldsymbol{V}_Y = (V_1, V_2, V_3)$, and the projected gradients $\mathbf{R}^T\nabla_{\boldsymbol{y}}V_j$, $j \in \{1,2,3\}$ are unique solutions in $L^2_\sharp(Y)^3$ of one of the following three problems $(\mathcal{K}_j)$ of electrostatic type (and similar problems for the local magnetic field):

$$(\mathcal{K}_j) : -\nabla_{\mathbf{R}}\cdot\Big[\varepsilon_r(\boldsymbol{y})\big(\nabla_{\mathbf{R}}(V_j(\boldsymbol{y}) - y_j)\big)\Big] = 0\ , \quad j \in \{1,2,3\}$$

IV. Conclusion

The paper analyzes a diffraction problem for irrational quasiperiodic metamaterials and develops a multiscale homogenization method with application to diffraction of photonic quasicrystals (PQs). The developed method can be used to compute remarkable diffractive properties of PQs.

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