Electromagnetic Homogenization: the Uncertainty Principle and Its Numerical Verification

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The effective permeability of electromagnetic metamaterials can deviate significantly from unity at high frequencies – an intriguing property not available in natural materials. However, we show both analytically and numerically that this artificial magnetism has limitations: the stronger the magnetic response, the less accurate the homogenization. New computational aspects of the paper include high-order Trefftz difference schemes and highly accurate computation of Bloch modes on nonorthogonal grids, high-order absorbing boundary conditions, and numerical implementation of new Trefftz homogenization on rhombic lattices.

Index Terms—**Composite materials, nonhomogeneous media, electromagnetic metamaterials, optical metamaterials, approximation methods, wave propagation, electrodynamics.**

I. Introduction

ONE of the most intriguing features of artificial periodic electromagnetic structures, known as metamaterials, is their nontrivial magnetic response, not available in natural media at high frequencies, and leading to remarkable phenomena, notably negative refraction and cloaking (see e.g. [1]). Much of the engineering and physical literature on the subject of metamaterials is devoted to their optimal (in some sense) design, whereby the effective material parameters attain a range of values desirable for specific applications – absorption, cloaking, lensing, etc. A tacit assumption is that there are no principal limitations on the achievable range of parameters, especially in the ideal case of negligible losses.

However, using our recently developed non-asymptotic homogenization theory [2], we show that such fundamental limits do exist. More specifically, the stronger the magnetic response (as measured by the deviation of the effective permeability tensor from identity), the less accurate ("certain") predictions of the effective medium theory are. We call this the *uncertainty principle* for the effective parameters of metamaterials.

II. Synopsis of the Non-Asymptotic Homogenization Theory

The homogenization problem under consideration consists in replacing a given periodic dielectric structure with an equivalent homogeneous body with a material tensor $\mathcal{M}$ to be determined. "Equivalence" is understood in the sense of transmission and reflection coefficients being approximately equal in the periodic and homogeneous cases within a given range of illumination conditions. For a detailed formulation of this problem, see [2].

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The homogenization procedure of [2] consists in (i) finding suitable approximations of fine-level (i.e. sub-cell) and coarse-level (coarser than the lattice cell size a) fields, and (ii) establishing a constitutive relationship between the pairs of coarse fields $(\mathbf{D}, \mathbf{B})$ and $(\mathbf{E}, \mathbf{H})$. No assumptions other than the intrinsic linearity of the constituent materials of the structure are made; in particular, anisotropy and magnetoelectric coupling may exist.

On both coarse and fine levels, we employ Trefftz approximations – i.e. approximations by functions satisfying the underlying equations and boundary conditions: e.g. Bloch waves on the fine level and plane waves on the coarse level. Trefftz functions have excellent approximation properties in many cases, even for bases of small size [5]–[8]

The end result of this analysis can be expressed in a particularly simple form if the tensor is known from symmetry considerations to be diagonal. Then, say, the xx component of the effective magnetic permeability is [2]

$$\mu_{xx} \; = \; \frac{\sum_\alpha (\mathbf{q}_\alpha \times [\mathbf{e}_\alpha])_x \, [h_{\alpha x}]^*}{k_0 \, \sum_\alpha \left| [h_{\alpha x}] \right|^2} \, , \tag{1}$$

where the asterisk denotes complex conjugation, k_0 is the wavenumber in free space, $\mathbf{q}$ is the Bloch vector of a basis wave, α is the index of the Bloch mode, $\mathbf{h}$ is the magnetic field of that mode, and square brackets denote surface averages of the tangential components of fields [2].

III. The Uncertainty Principle

Our theoretical analysis outlined above, along with a body of numerical evidence, lead to the following uncertainty principle for the magnetic response of intrinsically nonmagnetic periodic structures: *the stronger the magnetic effects in metamaterials, the less accurate the effective parameter representation*. In practice, there is still room for engineering design, but the

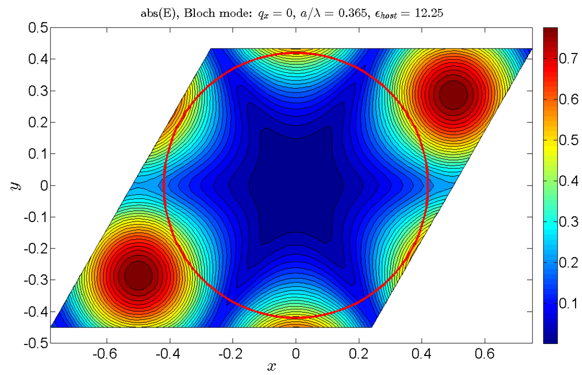

Fig. 1. Absolute value of E for the Bloch mode propagating to the right. Triangular lattice of cylindrical air holes from [10]. $a/\lambda = 0.365$ (close to the Γ-point in the second band). Red circle: air hole in a host dielectric.

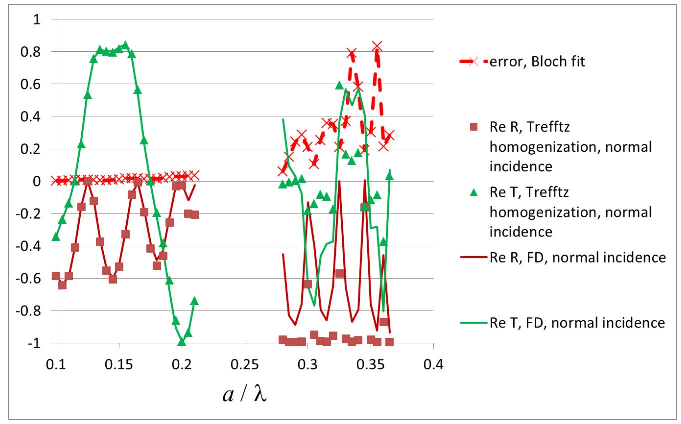

Fig. 2. Errors in the transmission and reflection coefficients, and the error δ_B of Bloch fit (see text) vs a/λ for the rhombic lattice of [10]. Large values of δ_B ("Bloch fit error") indicate an appreciable surface wave. $0.22 \lesssim a/\lambda \lesssim 0.28$ is the bandgap.

trade-offs between magnetic response and the accuracy of homogenization must always be borne in mind.

To avoid unnecessary technical complications, we assume that the material tensor is diagonal, in which case (1) applies. Straightforward algebra then shows that magnetic effects are due to higher-order harmonics of the Bloch wave, and therefore any methods relying only on the main Fourier harmonic of Bloch waves will not be able to reproduce these effects as a matter of principle. In other words, strong magnetic response (of intrinsically nonmagnetic structures) can only be observed if Bloch waves are significantly different from plane waves.

But it can be shown that the homogenization error also depends strongly on the same higher-order Bloch harmonics. Thus magnetic effects and homogenization errors go hand in hand, giving rise to the uncertainty principle.

IV. Numerical Examples

As an instructive example, we consider the triangular lattice of cylindrical air holes in a dielectric host, as investigated previously in [10]. The elementary cell of this lattice and the absolute value of the electric field of a Bloch wave are shown in Fig. 1. The radius of the hole is $r_{\text{cyl}} = 0.42a$, the dielectric permittivity of the host is $\epsilon_{\text{host}} = 12.25$; s-polarization (TM-mode, one-component E field perpendicular to the plane of the figure).

This example is interesting because it exhibits a particularly high level of isotropy around the Γ-point in the second photonic band.

Even in this highly isotropic case the uncertainty principle remains valid. First, isotropy with respect to the Bloch wavenumber is not accompanied by isotropy of the Bloch impedance (see [2], [9] for details on the latter). This leads to appreciable magnetoelectric coupling represented by the E-H_x and E-H_y terms in the 3×3 matrix $\mathcal{M}$ that relates (D, B_x, B_y) to (E, H_x, H_y). Even with this coupling, strong magnetic effects are accompanied by appreciable surface waves (SW) [2], [4], [11]. The magnitude of SW is evaluated via the difference δ_B (in the Euclidean norm) between an accurate (order six) finite difference solution of the full-scale wave propagation problem and its best approximation by Bloch waves. Large values of δ_B indicate the presence of an appreciable SW in addition to Bloch waves. As Fig. 2 shows, errors in the transmission and reflection coefficients (markers vs. solid lines) correlate strongly with δ_B (dashed line, crosses).

V. Conclusion

A non-asymptotic homogenization procedure is summarized and an uncertainty principle formulated: the stronger the magnetic response of periodic structures, the *less* accurate their homogenization. New computational features include high-order Trefftz difference schemes and highly accurate computation of Bloch modes on nonorthogonal grids, high-order absorbing boundary conditions, and numerical implementation of new Trefftz homogenization on rhombic lattices (details omitted due to the page limit but will be presented at the conference.)

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