Homogenization of Electromagnetic Metamaterials: Uncertainty Principles and a Fresh Look at Nonlocality

Igor Tsukerman

Department of Electrical and Computer Engineering,

The University of Akron, OH 44325-3904, USA

igor@uakron.edu

Joint work with Vadim Markel (University of Pennsylvania, USA & L'Institut Fresnel – Aix Marseille Université, France)

Homogenization of Electromagnetic Metamaterials: Uncertainty Principles and a Fresh Look at Nonlocality

Igor Tsukerman

Department of Electrical and Computer Engineering,

The University of Akron, OH 44325-3904, USA

igor@uakron.edu

Joint work with Vadim Markel (University of Pennsylvania, USA & L'Institut Fresnel – Aix Marseille Université, France)

Collaborators

Vadim Markel (University of Pennsylvania, USA)

Xiaoyan Xiong, Li Jun Jiang (Hong Kong University)

I sincerely thank the organizers (Prof. Che Ting Chan and others) for the kind invitation.

Outline

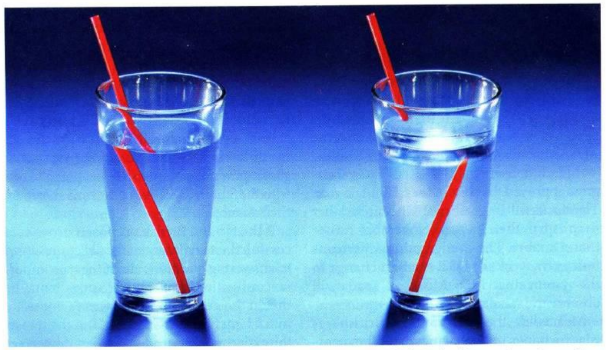
- Overview
  - Established theories
  - Pitfalls
- Non-asymptotic homogenization
- Uncertainty principles
- Nonlocal homogenization

Metamaterials and “Optical Magnetism”

D.R. Smith *et al.*, 2000

- Artificial periodic structures with geometric features smaller than the wavelength.
- Usually contain resonating entities.
- Controlling the flow of waves.
- Appreciable magnetic effects possible at high frequencies.
- Effective parameters essential for design.

E. SCHREMPP/SPL



A straw in a glass of water seems disjointed because of refraction (left). But in this rough mock-up of what would happen if water had a negative refractive index (right), the effect is startling. The underside of the water's surface can be seen but not the bottom of the glass. For more accurate models, see ref. 4.

Nature, 1/25/07

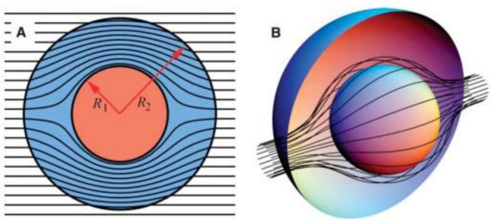


Fig. 2. A ray-tracing program has been used to calculate ray trajectories in the cloak, assuming that $R_2 \gg \lambda$. The rays essentially following the Poynting vector. (**A**) A two-dimensional (2D) cross section of rays striking our system, diverted within the annulus of cloaking material contained within $R_1 < r < R_2$ to emerge on the far side undeviated from their original course. (**B**) A 3D view of the same process.

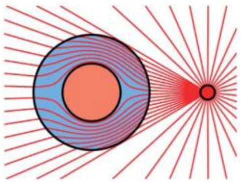
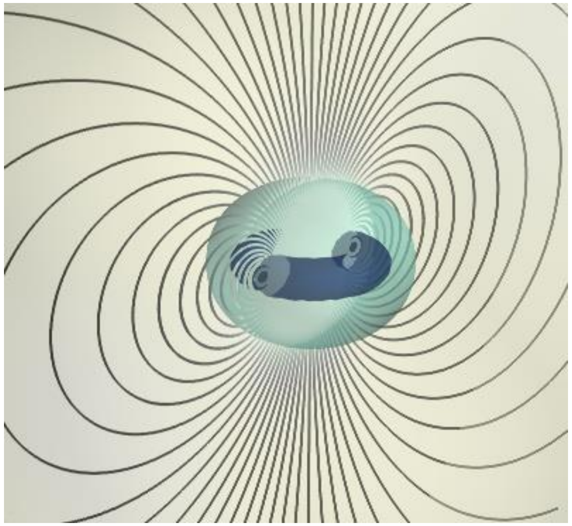


Fig. 3. A point charge located near the cloaked sphere. We assume that $R_2 \ll \lambda$, the near-field limit, and plot the electric displacement field. The field is excluded from the cloaked region, but emerges from the cloaking sphere undisturbed. We plot field lines closer together near the sphere to emphasize the screening effect.

www.sciencemag.org SCIENCE VOL 312 23 JUNE 2006 1781

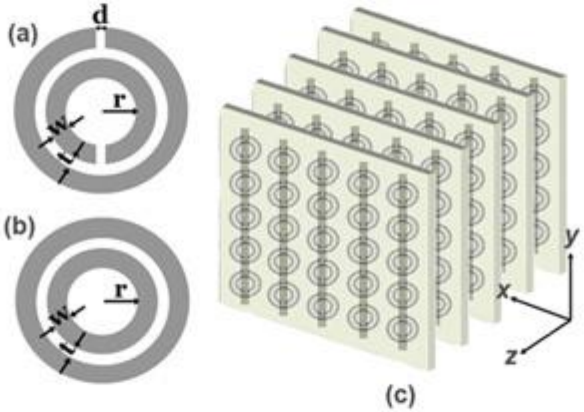
Pendry, Schurig & Smith, Science 2006

Traditional Viewpoint: Dipoles and Resonances



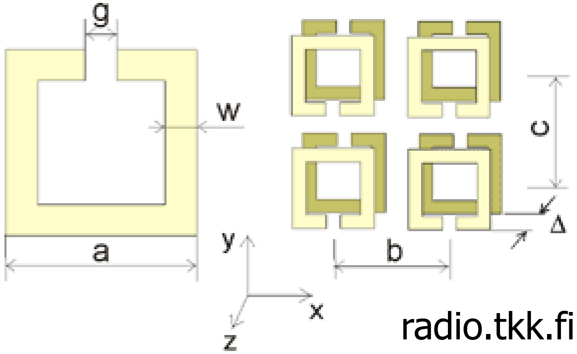
http://staging.enthought.com

$$\nabla \times \mathbf{e} = i\omega c^{-1}\mathbf{b}, \quad \nabla \times \mathbf{b} = -i\omega c^{-1}\mathbf{d}$$



www.fen.bilkent.edu.tr/~aydin

Split rings → "LC" resonances
→ magnetic dipoles



radio.tkk.fi

Homogenization

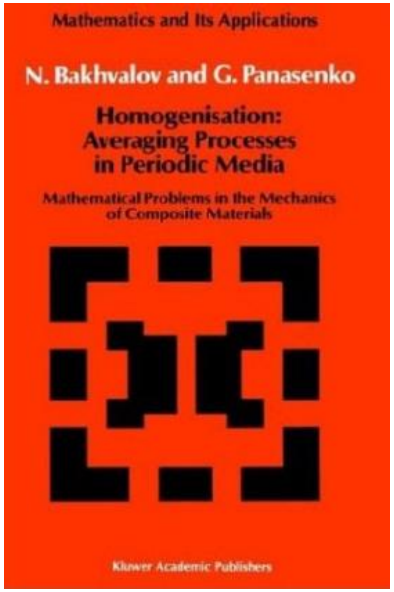
Characterize a periodic structure by equivalent effective ("macroscopic", coarse-scale) parameters.

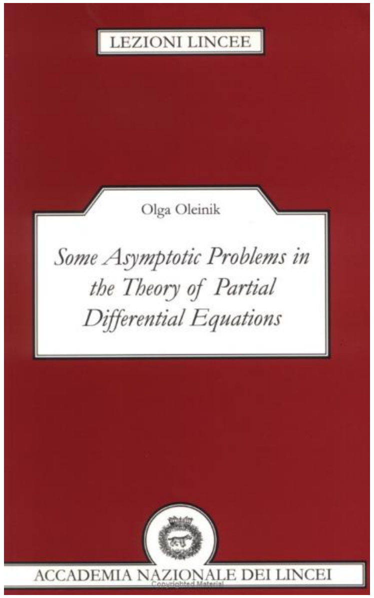
[Details to follow.]

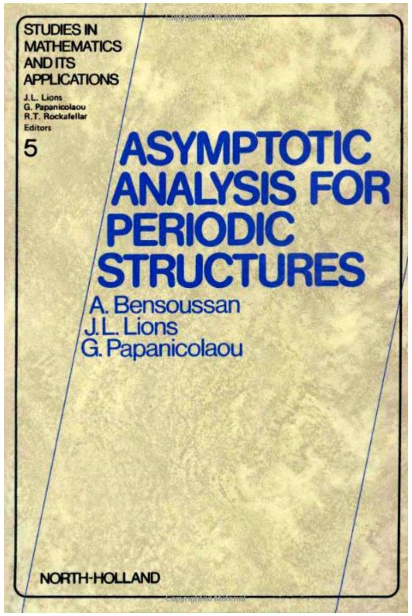
Well-established Asymptotic Theories

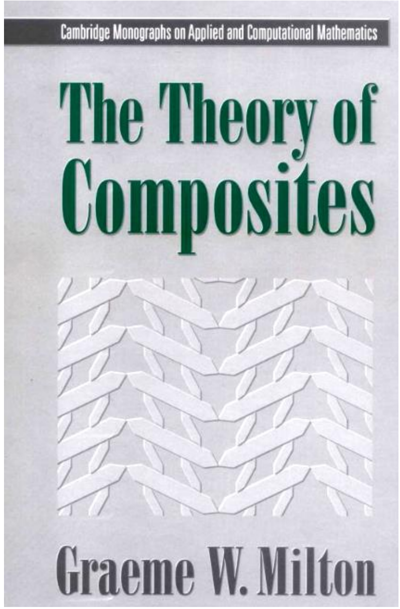
Classical effective medium theories and their extensions:

Mossotti (1850), Lorenz (1869), Lorentz (1878), Clausius (1879), Maxwell Garnett (1904), Lewin (1947), Khizhnyak (1957, 59), Waterman & Pedersen (1986).









Many books (physical & mathematical); ~24,000 papers.

SIAM J. MATH. ANAL.
Vol. 23, No. 6, pp. 1482–1518, November 1992

HOMOGENIZATION AND TWO-SCALE CONVERGENCE*

GRÉGOIRE ALLAIRE†

L_ε (with coefficients oscillating with period ε), and a family of solutions u_ε which, for a given domain Ω and source term f, satisfy

$$L_\varepsilon u_\varepsilon = f \quad \text{in } \Omega, \tag{0.1}$$

complemented by appropriate boundary conditions. Assuming that the sequence u_ε converges, in some sense, to a limit u, we look for a so-called homogenized operator $\bar{L}$ such that u is a solution of

$$\bar{L}u = f \quad \text{in } \Omega. \tag{0.2}$$

Passing from (0.1) to (0.2) is the homogenization process. (There is a vast body of literature on that topic; see [10], [40] for an introduction, and additional references.) Although homogenization is not restricted to the case of periodically oscillating operators (cf. the Γ-convergence of DeGiorgi [16], [17], the H-convergence of Tartar [42], [34], or the G-convergence of Spagnolo [41], [49]), we restrict our attention to that particular case. This allows the use of the well known two-scale asymptotic expansion method [7], [10], [27], [40] in order to find the precise form of the homogenized operator $\bar{L}$. The key to that method is to postulate the following ansatz for u_ε:

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \cdots, \tag{0.3}$$

where each term $u_i(x, y)$ is periodic in y. Then, inserting (0.3) in (0.1) and identifying powers of ε leads to a cascade of equations for each term u_i. In general, averaging with respect to y that for u_0 gives (0.2), and the precise form of $\bar{L}$ is computed with the help of a so-called cell equation in the unit period (see [10], [40] for details). This method is very simple and powerful, but unfortunately is formal since, a priori, the ansatz (0.3) does not hold true. Thus, the two-scale asymptotic expansion method is used only to guess the form of the homogenized operator $\bar{L}$, and other arguments are needed to prove the convergence of the sequence u_ε to u. To this end, the more general and powerful method is the so-called energy method of Tartar [42]. Loosely speaking, it amounts to multiplying equation (0.1) by special test functions (built with the solutions of the cell equation), and passing to the limit as $\varepsilon \to 0$. Although products of weakly convergent sequences are involved, we can actually pass to the limit thanks to some "compensated compactness" phenomenon due to the particular choice of test functions.

When asymptotic theories are not sufficient:

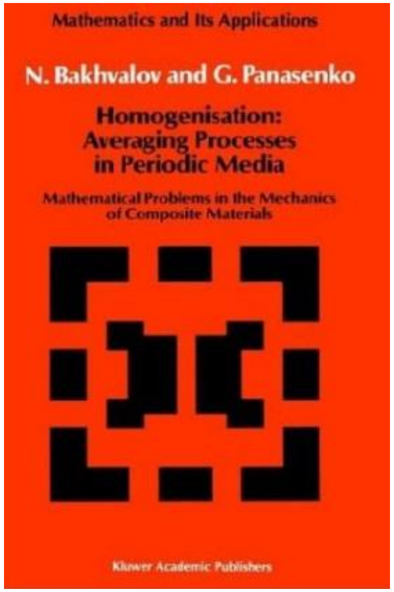
some pitfalls

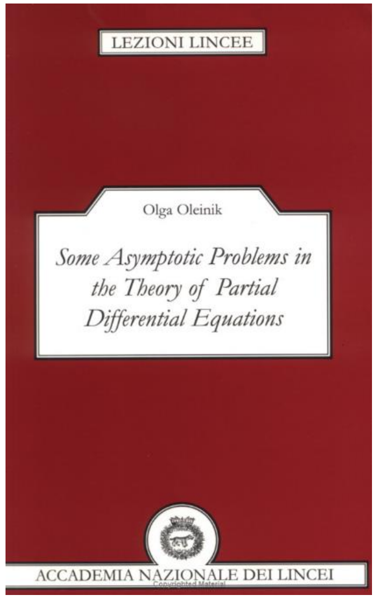
Some Pitfalls: zero cell size limit

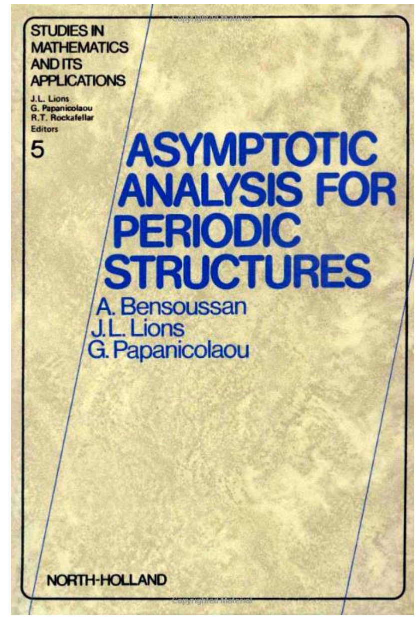
- Metamaterials: cell size smaller than the vacuum wavelength but not vanishingly small. (Typical ratio ~0.1−0.3.)
- This is a principal limitation, not just a fabrication constraint (Sjoberg et al. *Multiscale Mod & Sim*, 2005; Bossavit et al, *J. Math. Pures & Appl*, 2005; IT, *JOSA B*, 2008).
- Cell size $a \to 0$: nontrivial physical effects (e.g.“artificial magnetism”) disappear.

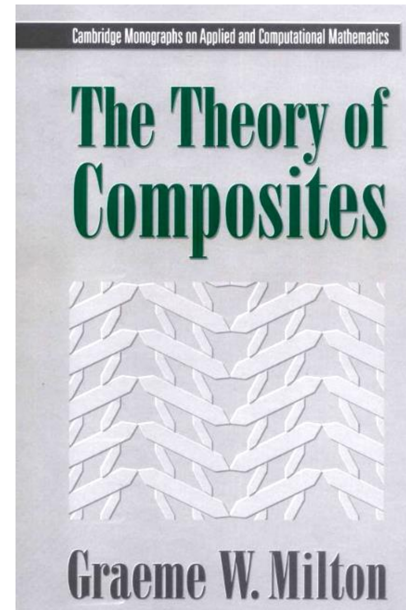
Classical effective medium theories and their extensions:

Mossotti (1850), Lorenz (1869), Lorentz (1878), Clausius (1879), Maxwell Garnett (1904), Lewin (1947), Khizhnyak (1957, 59), Waterman & Pedersen (1986).









~~Zero cell size limit~~

Non-asymptotic homogenization, local and nonlocal

Pitfalls in Homogenization: Bulk Behavior

- Even for infinite isotropic homogeneous media, only the product εμ is uniquely defined; impedance is not!
- Indeed, Maxwell's equations are invariant w.r.t. rescaling **H** $\to \gamma$**H**, **D** $\to \gamma$**D**:

$$\nabla \times \mathbf{E} = i\omega c^{-1}\mathbf{B} \qquad \nabla \times \mathbf{H} = -i\omega c^{-1}\mathbf{D}$$

- $\mathbf{J} = \partial_t \mathbf{P} + c\nabla\times\mathbf{M}$: decomposition not unique
- $\Rightarrow$ Bulk behavior alone does not define effective parameters. Must consider boundaries!

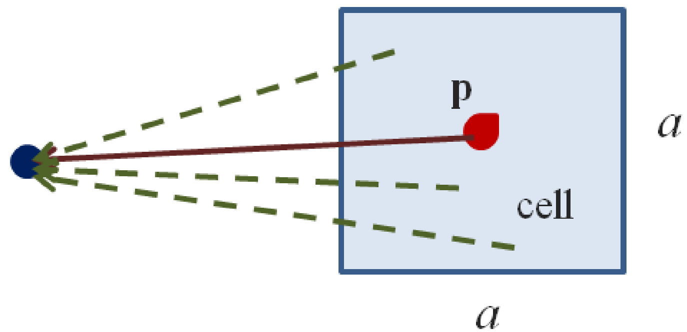
Felbacq, J. Phys. A 2000; Lawrence *et al*. Adv. Opt. Photon. 2013;
IT, JOSA B, 2011; VM & IT, Phys. Rev. B 88, 2013;
VM & IT, Proc Royal Soc A 470, 2014.

Bulk behavior alone does not define effective parameters?

But wait…
what about **M** in the bulk (“dipole moment per unit volume”)?

What about **M** in the bulk ("dipole moment per unit volume")?

- This textbook concept works because of the far field approximation *outside a finite body*.
- If a small inclusion, approximated as an ideal dipole, is replaced with a distributed moment, the error in the far field is $\mathcal{O}((ka)^2)$. But magnetic effects are also of order $\mathcal{O}((ka)^2)$!



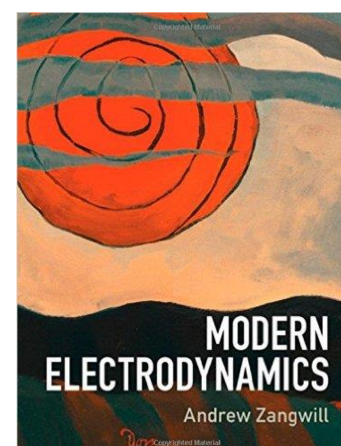
“Dipole moment per unit volume” continued

- Defining “dipole moment p.u.v.” $\mathbf{M}(\mathbf{r})$ in such a way that $c\nabla\times\mathbf{M}(\mathbf{r}) = \mathbf{J}(\mathbf{r})$ for a general current distribution is not at all easy.
- For example, try $\mathbf{M} = \dfrac{1}{2c}\mathbf{r}\times\mathbf{J}$:

$$c\,(\nabla\times\,\mathbf{M})_x = \frac{x}{2}\frac{\partial J_y}{\partial y} - \frac{y}{2}\frac{\partial J_x}{\partial y} + \frac{x}{2}\frac{\partial J_z}{\partial z} - \frac{z}{2}\frac{\partial J_x}{\partial z} - J_x \neq J_x$$

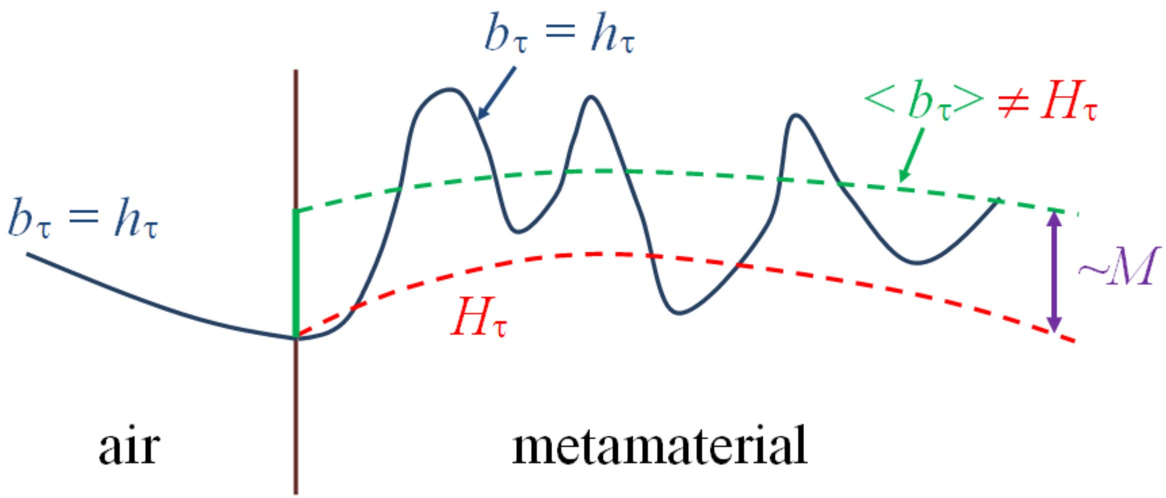
- Mollifying does not help:

$$c\,\nabla\times(\mathbf{M}*w) = c\,(\nabla\times\,\mathbf{M})*w \neq \mathbf{J}*w$$



The Role of Boundaries (physical intuition)

Consider e.g. the tangential component of the magnetic field



- On the fine scale, **b** = **h**.

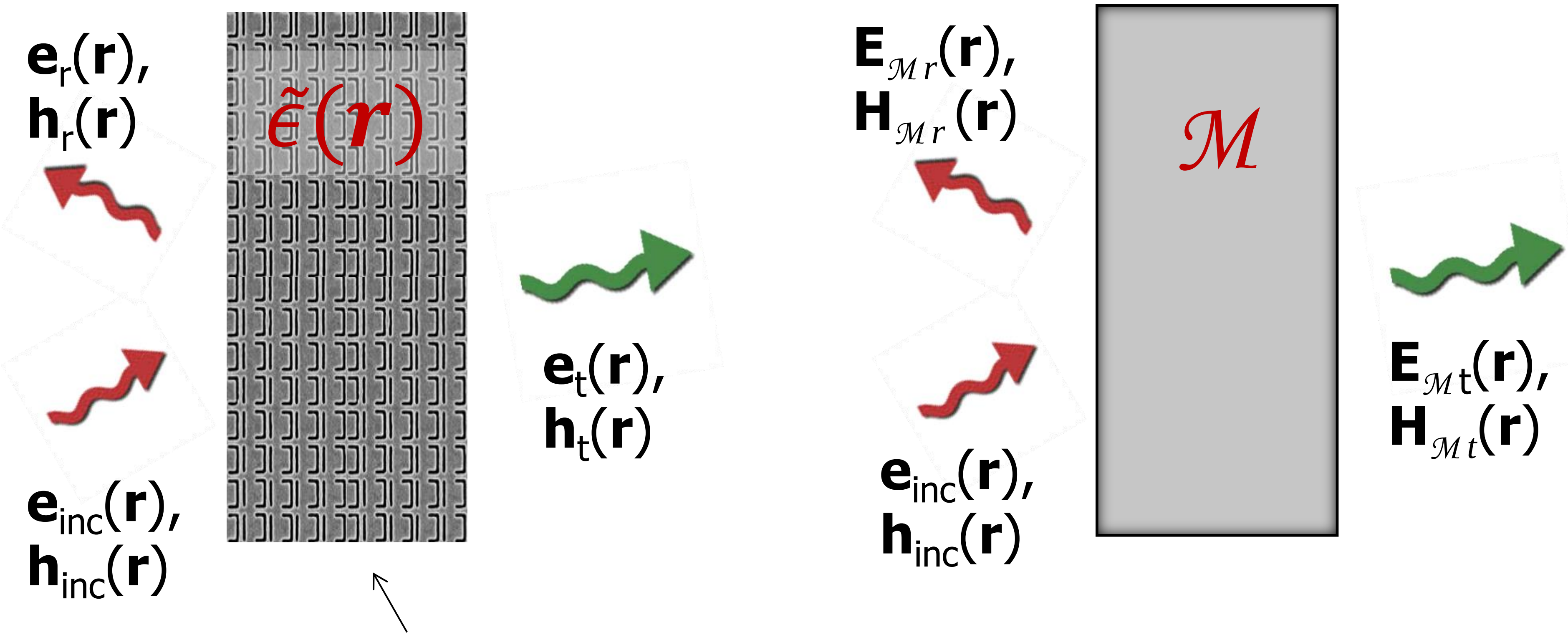
IT, *JOSA B*, 2011.

- Volume averaging of **b** leads (in general) to a jump at the boundary. But H_τ must be continuous. Otherwise – nonphysical artifacts (spurious boundary sources).

$$\mathbf{E}, \mathbf{H} \in H(\mathrm{curl}, \Omega); \quad \mathbf{B}, \mathbf{D} \in H(\mathrm{div}, \Omega)$$

Non-Asymptotic Homogenization

- Periodic vs. homogeneous material: match TR as accurately as possible.
- From b.c.: EH-amplitudes of plane waves must be surface averages of Bloch waves.
- From Maxwell's equations: DB-amplitudes follow from the EH-amplitudes.



Credit: www.orc.soton.ac.uk
(part of the image)

Non-asymptotic homogenization

- Compare: TR from a metamaterial slab vs. a homogeneous slab.
- Bloch modes vs. generalized plane waves.
- **EH** amplitudes of plane waves determined from boundary conditions.
- **DB** amplitudes then found from the Maxwell curl equations.
- The material tensor is found as **DB** "divided" by **EH** (in the least squares sense).

PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

A non-asymptotic homogenization theory for periodic electromagnetic structures

Igor Tsukerman and Vadim A. Markel

Proc. R. Soc. A 2014 **470**, 20140245, published 28 May 2014

Approximation of Fine-Scale Fields

$$\psi(\mathbf{r}) = \sum_{\alpha, m} c_{m\alpha} \psi_{m\alpha}(\mathbf{r}) + \delta(\mathbf{r}),$$

δ: 'out-of-the-basis' error (assumed small).
m – lattice cell index
ψ – Trefftz basis
Homogenization relies only on basis $\{\psi\}$, not coefficients *c*.

Assume Bloch wave basis

$$\mathbf{e}_\alpha(\mathbf{r}) = \tilde{\mathbf{e}}_\alpha(\mathbf{r}) \exp(\mathrm{i}\mathbf{q}_\alpha \cdot \mathbf{r}) \quad \text{and} \quad \mathbf{h}_\alpha(\mathbf{r}) = \tilde{\mathbf{h}}_\alpha(\mathbf{r}) \exp(\mathrm{i}\mathbf{q}_\alpha \cdot \mathbf{r}),$$

Coarse-Level Bases

- Plane-wave solutions Maxwell's equations in a homogeneous but possibly anisotropic medium:

$$\Psi(\mathbf{r}) = \sum_{\alpha} c_{m\alpha} \Psi_{m\alpha}(\mathbf{r}) \quad \text{and} \quad \Psi_{m\alpha}(\mathbf{r}) \equiv \{\mathbf{E}^{(0)}_{m\alpha}, \mathbf{H}^{(0)}_{m\alpha}\} \exp(i\mathbf{q}_{m\alpha} \cdot \mathbf{r}), \quad \mathbf{r} \in \mathbb{C}_m$$

- The amplitudes $\{\mathbf{E}^{(0)}_{m\alpha}, \mathbf{H}^{(0)}_{m\alpha}\}$ are yet to be determined.

Coarse-Scale Fields

Satisfy Maxwell's equations with an effective material tensor approximately but accurately:

$$\delta \mathrm{J}_m(\mathrm{r}) = \nabla \times \mathrm{H}(\mathrm{r}) + ik_0 \mathrm{D}(\mathrm{r}), \quad \mathrm{r} \in \mathbb{C}_m,$$

$$\delta \mathrm{I}_m(\mathrm{r}) = \nabla \times \mathrm{E}(\mathrm{r}) - ik_0 \mathrm{B}(\mathrm{r}), \quad \mathrm{r} \in \mathbb{C}_m,$$

$$\delta \mathrm{K}_{lm}(\mathrm{r}) = \hat{\mathrm{n}}_{lm} \times [\mathrm{H}_l(\mathrm{r}) - \mathrm{H}_m(\mathrm{r})], \quad \mathrm{r} \in \mathbb{S}_{lm},$$

$$\delta \mathrm{Q}_{lm}(\mathrm{r}) = \hat{\mathrm{n}}_{lm} \times [\mathrm{E}_l(\mathrm{r}) - \mathrm{E}_m(\mathrm{r})], \quad \mathrm{r} \in \mathbb{S}_{lm}$$

$$\{\mathrm{D}(\mathrm{r}), \mathrm{B}(\mathrm{r})\} = \begin{cases} \mathcal{M}_m\{\mathrm{E}(\mathrm{r}), \mathrm{H}(\mathrm{r})\}, & \mathrm{r} \in \mathbb{C}_m, \\ \{\mathrm{E}(\mathrm{r}), \mathrm{H}(\mathrm{r})\}, & z \notin [0, L], \end{cases}$$

The δ-terms can be interpreted as spurious volume and surface currents representing approximation errors.

Minimizing the Interface Error

- Minimize, for each cell boundary, the discrepancy between the coarse fields and the respective fine-scale fields:

$$\min_{\mathbf{E}^{(0)}_{m\alpha},\mathbf{H}^{(0)}_{m\alpha}} \{\|\hat{\mathbf{n}} \times (\mathbf{E}_{m\alpha} - \mathbf{e}_{m\alpha})\|_{\partial\mathbb{C}_m} + \|\hat{\mathbf{n}} \times (\mathbf{H}_{m\alpha} - \mathbf{h}_{m\alpha})\|_{\partial\mathbb{C}_m}\},$$

- For hexahedral cells,

$$\mathbf{E}^{(0)}_{m\alpha x} = \int_{\partial\mathbb{C}_{mx}} \tilde{\mathbf{e}}_{m\alpha x}\, \mathrm{d}S \quad \text{and} \quad \mathbf{H}^{(0)}_{m\alpha x} = \int_{\partial\mathbb{C}_{mx}} \tilde{\mathbf{h}}_{m\alpha x}\, \mathrm{d}S,$$

  ∂C_{mx} – four faces parallel to the *x*-axis.

- Note that the averages above involve the periodic factor of the Bloch wave.

Minimizing the Volume Error

$$\min_{\mathcal{M}_m} \sum_{\alpha} \|\mathcal{K}_{m\alpha}\{\mathrm{H}^{(0)}_{m\alpha}, \mathrm{E}^{(0)}_{m\alpha}\} - k_0 \mathcal{M}_m \{\mathrm{E}^{(0)}_{m\alpha}, \mathrm{H}^{(0)}_{m\alpha}\}\|^2$$

$$\mathcal{K}_{m\alpha} \equiv \begin{pmatrix} -\mathrm{q}_{m\alpha}\times & 0 \\ 0 & \mathrm{q}_{m\alpha}\times \end{pmatrix}$$

- $\mathbf{q}\times$ is the matrix representation of the cross product with $\mathbf{q}$
- This problem has a closed-form solution for the material tensor because the functional is quadratic with respect to the entries of $\mathcal{M}$.

The Algebraic System

$$
\begin{array}{|c|c|}\hline \varepsilon & \xi \\ \hline \zeta & \mu \\ \hline \end{array}
\times
\begin{array}{r|c|c|c|c|c|}
 & \text{Basis wave 1} & \text{Basis wave 2} & \ldots & \ldots & \text{Basis wave } N \\
 & \downarrow & \downarrow & & & \downarrow \\ \hline
\mathbf{E}_0 \rightarrow & & & & & \\ \hline
\mathbf{H}_0 \rightarrow & & & & & \\ \hline
\end{array}
\overset{\text{l.s.}}{=}
$$

$6 \times N$

6×6 tensor to be found

$\mathbf{E}_0$, $\mathbf{H}_0$ for each basis wave found from interface b.c.

$$
\begin{array}{r|c|c|c|c|c|}
 & \text{Basis wave 1} & \text{Basis wave 2} & \ldots & \ldots & \text{Basis wave } N \\
 & \downarrow & \downarrow & & & \downarrow \\ \hline
\mathbf{D}_0 \rightarrow & & & & & \\ \hline
\mathbf{B}_0 \rightarrow & & & & & \\ \hline
\end{array}
$$

$6 \times N$

$\mathbf{D}_0$, $\mathbf{B}_0$ for each basis wave found from the Maxwell curl equations

The Case of Diagonal Tensors

$$\epsilon_{m,xx} = \frac{\sum_\alpha (\mathbf{q}_{m\alpha} \times [\mathbf{h}_{m\alpha}])_x [e_{m,\alpha x}]^*}{k_0 \sum_\alpha |[e_{m,\alpha x}]|^2},$$

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

- Physical interpretation: ensemble averages of Bloch impedances of the basis waves.
- The physical significance of Bloch impedance has been previously emphasized by other researchers (Simovski 2009, Lawrence *et al.* 2013).

Non-Diagonal Tensor

$$\mathcal{M}_{m,\mathrm{opt}} = \arg\min_{\mathcal{M}} F_m(\mathcal{M}) \quad \text{and} \quad F_m(\mathcal{M}) \equiv \| \Psi_{m,DB} - \mathcal{M}\Psi_{m,EH} \|$$

$$\mathcal{M}_{m,\mathrm{opt}} = \Psi_{m,DB}\Psi^{+}_{m,EH}$$

$\Psi_{\mathrm{m,DB}}$ and $\Psi_{\mathrm{m,EH}}$: $6 \times n$ matrices with columns α $\quad k_0^{-1}\mathcal{K}_{m\alpha}\{\mathbf{H}^{(0)}_{m\alpha}, \mathbf{E}^{(0)}_{m\alpha}\}$ and $\{\mathbf{E}^{(0)}_{m\alpha}, \mathbf{H}^{(0)}_{m\alpha}\}$

PROCEEDINGS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

A non-asymptotic homogenization theory for periodic electromagnetic structures

Igor Tsukerman and Vadim A. Markel

Proc. R. Soc. A 2014 **470**, 20140245, published 28 May 2014

Error indicator:

$$\chi = \max_{m}[F_m(\mathcal{M}_{m,\mathrm{opt}})]$$

Now focus on the “uncertainty principle”: the stronger the magnetic response, the less accurate (“certain") the predictions of the effective medium theory.

IT and Vadim Markel, Nonasymptotic homogenization of periodic electromagnetic structures: Uncertainty principles, PRB 93, 024418, 2016.

Vadim Markel and IT, Can photonic crystals be homogenized in higher bands? arxiv.org:1512.05148, submitted.

Fields in the metamaterial (s-mode)

A Bloch wave

$$e_B(\mathbf{r},\mathbf{q}) \;=\; E_B\tilde{e}_B(\mathbf{r})\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r})$$

The tangential component of **h**

$$h_\tau(\mathbf{r}) \;=\; \frac{1}{\mathrm{i}k_0}\frac{\partial e}{\partial n} \;=\; E_B\tilde{h}_{B\tau}(\mathbf{r})\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r})$$

$$\tilde{h}_{B\tau}(\mathbf{r}) \;=\; \frac{q_n}{k_0}\;\tilde{e}_B + \frac{1}{\mathrm{i}k_0}\frac{\partial\tilde{e}_B}{\partial n}$$

Fields in the air

$$e_{\mathrm{air}}(\mathbf{r}) \;=\; E_{\mathrm{inc}}\left(\exp(\mathrm{i}\mathbf{k}_{\mathrm{inc}}\cdot\mathbf{r}) + R\exp(\mathrm{i}\mathbf{k}_{\mathrm{r}}\cdot\mathbf{r})\right)$$

$$h_{\mathrm{air},\tau}(\mathbf{r}) \;=\; E_{\mathrm{inc}}\cos\theta_{\mathrm{inc}}\left(\exp(\mathrm{i}\mathbf{k}_{\mathrm{inc}}\cdot\mathbf{r}) - R\exp(\mathrm{i}\mathbf{k}_{\mathrm{r}}\cdot\mathbf{r})\right)$$

Fields in the equivalent material

A plane wave

$$E_{\mathrm{T}}(\mathbf{r}) \;=\; E_{\mathrm{T}0}\exp(\mathrm{i}\mathbf{k}_{\mathrm{T}}\cdot\mathbf{r})$$

$$H_{\mathrm{T}\tau}(\mathbf{r}) \;=\; H_{\mathrm{T}\tau 0}\exp(\mathrm{i}\mathbf{k}_{\mathrm{T}}\cdot\mathbf{r})$$

$$\mathbf{k}_{\mathrm{T}} \;=\; \mathbf{q}$$

What should the EHDB-amplitudes of the plane wave be for best approximation?

What should the EHDB-amplitudes be?

Interface boundary conditions $\Rightarrow$ E, H amplitudes:

$$E_{\mathrm{T}0} = E_B \langle \tilde{e}_B \rangle_S \qquad (= (1+R)E_{\mathrm{inc}})$$

$$H_{\mathrm{T}\tau 0} = E_B \langle \tilde{h}_B \rangle_S$$

Maxwell's equations inside the material $\Rightarrow$ B, D amplitudes:

$$B_{\mathrm{T}\tau 0} = \frac{q_n}{k_0} E_B \langle \tilde{e}_B \rangle_S$$

For cells with mirror symmetry,

$$\zeta_{\tau\tau} \equiv 1 - \mu_{\tau\tau}^{-1} = \frac{\mathrm{i}\,\langle \partial_n e_\sim \rangle_S}{q\cos\theta_B (e_0 + \langle e_\sim \rangle_S)}$$

$$\tilde{e}_B \equiv e_0 + e_\sim, \quad e_0 = \mathrm{const}, \quad \int_C e_\sim \, dC = 0$$

$$\zeta_{\tau\tau} \equiv 1 - \mu_{\tau\tau}^{-1} = \frac{\mathrm{i}\,\langle \partial_n e_{\sim} \rangle_S}{q \cos\theta_B (e_0 + \langle e_{\sim} \rangle_S)}$$

Magnetic effects in metamaterials are due entirely to higher-order spatial harmonics of the Bloch wave.

It is qualitatively clear that the angular dependence of $\zeta_{\tau\tau}$ will tend to be stronger when the magnetic effects (nonzero $\zeta_{\tau\tau}$) are themselves stronger, as both are controlled by $e_{\sim}$.

This conclusion can also be supported quantitatively.

VM & IT, Nonasymptotic Homogenization of Periodic Electromagnetic Structures: an Uncertainty Principle, to appear in Phys Rev B, 2016.

A Numerical Example

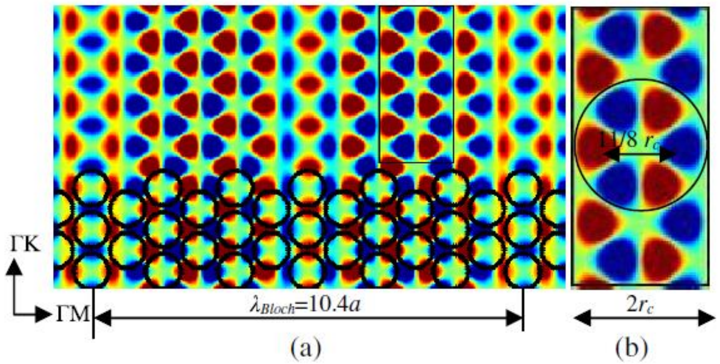
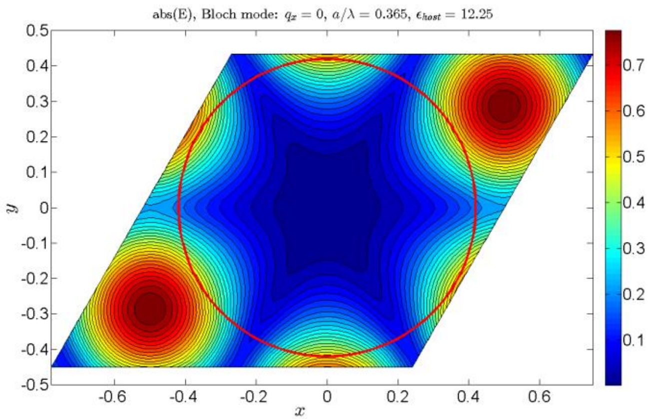
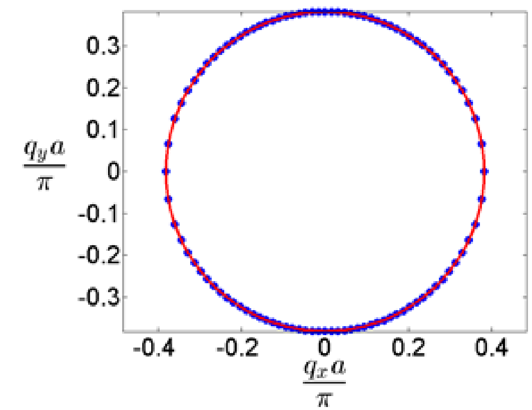


Fig. 2. (Color online) (a) E_z-field distribution of the TM-polarization Bloch wave with frequency 0.36(c/a) in a 2D triangular PhC. Some air holes are denoted as black circles; (b) Field distribution of the rectangular region in (a). Each unit can be covered by a circle.



Hex lattice of cylindrical air holes in a dielectric host (Pei & Huang, *JOSA B*, 29, 2012). Radius of the hole: 0.42a. Dielectric permittivity of the host: 12.25. s-polarization (TM-mode).

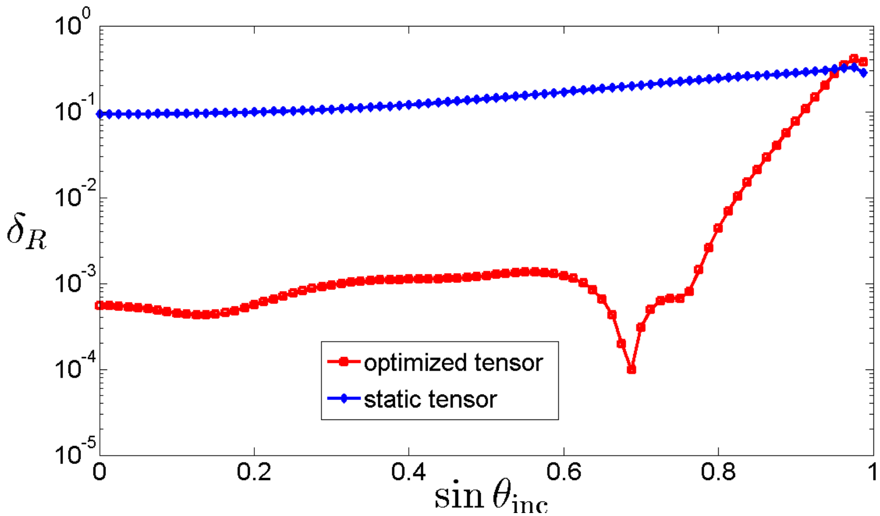
The second photonic band it exhibits a high level of isotropy around the Γ-point and a negative effective index.



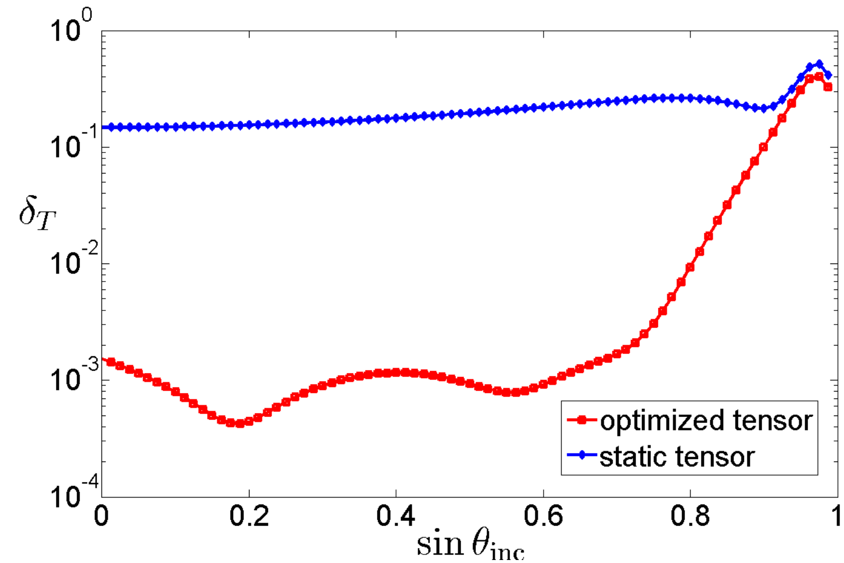
Isofrequency contour almost circular at $a = 0.365\lambda$ (near 2nd Γ–point $a \approx 0.368\lambda$).

Numerical Features

- Flexible Local Approximation Method (FLAME), high-order Trefftz-FD schemes:
  - IT, *J Comp Phys* 2006, *IEEE Trans Mag* 2005, 2008.
  - IT, Springer, 2007.
- FLAME on rhombic grids for Bloch modes.
- General motif: Trefftz methods.
- Material tensor for optimal fit to the TR data, using Matlab's `fminsearch`.

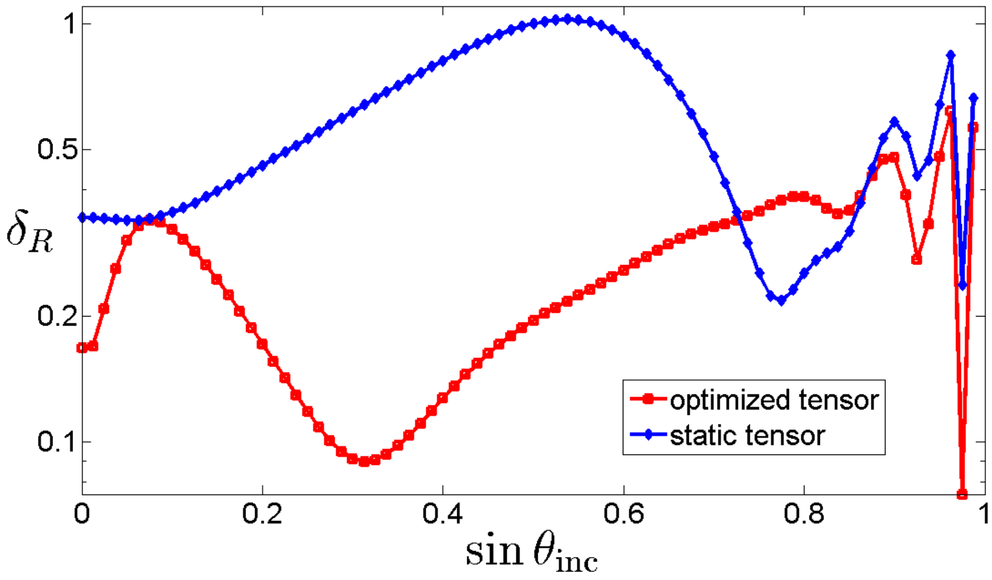


$a = 0.1\lambda$

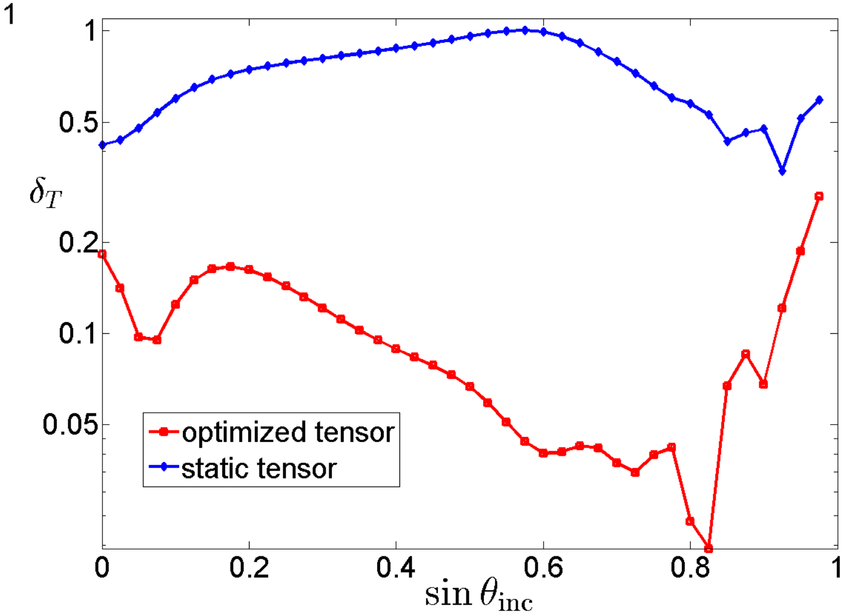


IT and Vadim Markel, Nonasymptotic homogenization of periodic electromagnetic structures: Uncertainty principles, arxiv.org:11510.05002, PRB 2016.

Absolute errors in R (left) and T (right) as functions of the sine of the angle of incidence. Tensor optimization was performed within the range [0, π/4] for the angle of incidence. Hex lattice of cylindrical air holes in a dielectric host (Pei & Huang).



$a = 0.365\lambda$



IT and Vadim Markel, Nonasymptotic homogenization of periodic electromagnetic structures: Uncertainty principles, arxiv.org:11510.05002, PRB 2016.

Same but for $a = 0.365\lambda$. Stronger magnetic effects – poorer homogenization accuracy.

From non-asymptotic to nonlocal theory

Recall Local Approximation First

$$
\begin{bmatrix} \varepsilon & \xi \\ \zeta & \mu \end{bmatrix}
\times
\begin{array}{c}
\\
\mathbf{E}_0 \rightarrow \\
\mathbf{H}_0 \rightarrow
\end{array}
\begin{array}{ccccc}
\text{Basis wave 1} & \text{Basis wave 2} & \ldots & \ldots & \text{Basis wave } N \\
\downarrow & \downarrow & & & \downarrow
\end{array}
\underbrace{\begin{bmatrix} \; & \; & \; & \; & \; \\ \; & \; & \; & \; & \; \end{bmatrix}}_{6 \times N}
\overset{\text{l.s.}}{=}
$$

6 × 6 tensor to be found

E$_0$, **H**$_0$ for each basis wave found from interface b.c.

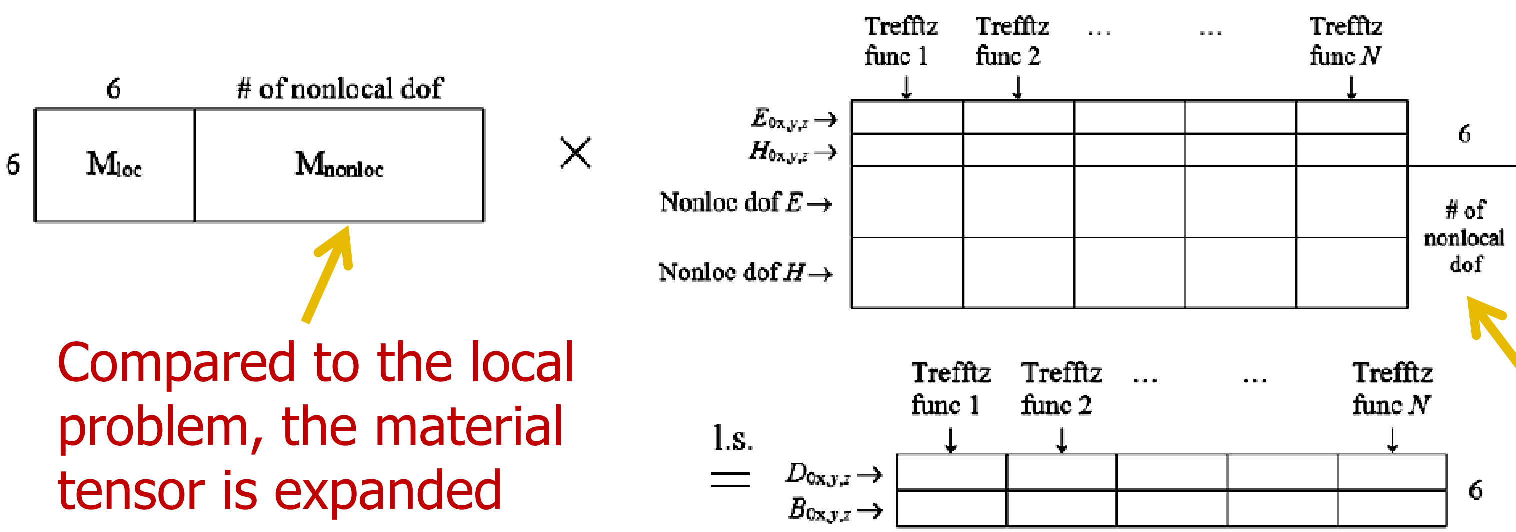
$$
\begin{array}{c}
\\
\mathbf{D}_0 \rightarrow \\
\mathbf{B}_0 \rightarrow
\end{array}
\begin{array}{ccccc}
\text{Basis wave 1} & \text{Basis wave 2} & \ldots & \ldots & \text{Basis wave } N \\
\downarrow & \downarrow & & & \downarrow
\end{array}
\underbrace{\begin{bmatrix} \; & \; & \; & \; & \; \\ \; & \; & \; & \; & \; \end{bmatrix}}_{6 \times N}
$$

D$_0$, **B**$_0$ for each basis wave found from the dispersion relations

A Nonlocal Model

$$\min_{\mathcal{M}_m, \mathcal{M}_{m,\mathrm{nonlocal}}} \sum_{\alpha} \left\| \mathcal{K}_{m\alpha}\{\mathbf{H}^{(0)}_{m\alpha}, \mathbf{E}^{(0)}_{m\alpha}\} - k_0 \mathcal{M}_m \{\mathbf{E}^{(0)}_{m\alpha}, \mathbf{H}^{(0)}_{m\alpha}\} - k_0 \mathcal{M}_{m,\mathrm{nonlocal}} \{\mathbf{E}^{(0)}_{m\alpha}, \mathbf{H}^{(0)}_{m\alpha}, \eta\} \right\|^2$$

η is a vector of additional (nonlocal, integral) degrees of freedom (dof) for the coarse-level field.



Compared to the local problem, the material tensor is expanded "rightward"

The EH-matrix is expanded "downward," with additional **E** and **H** dof.

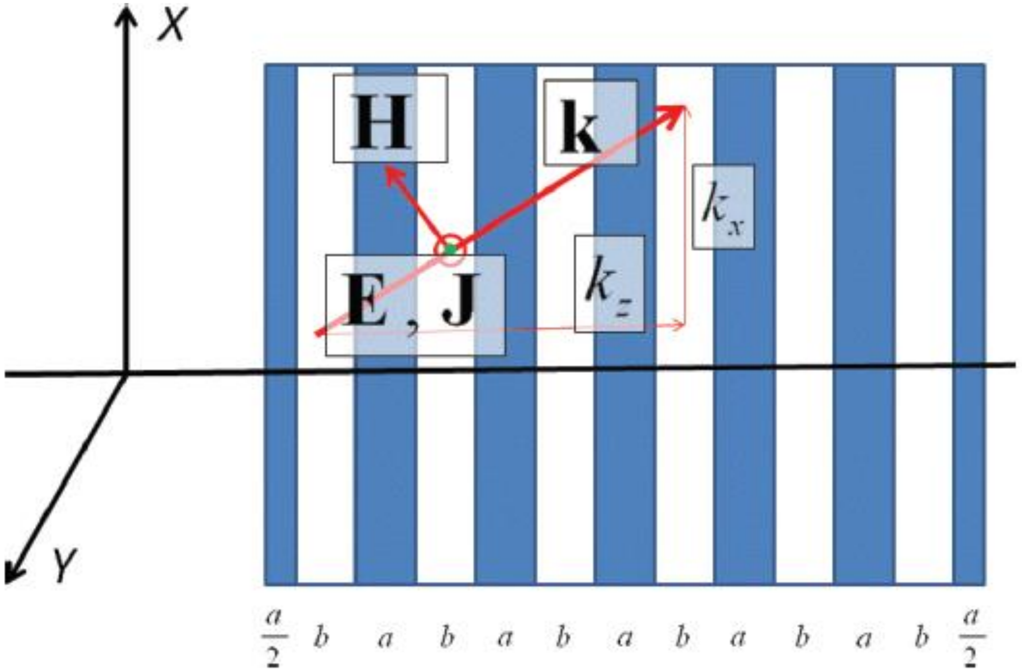
Numerical Example: Layered Media

- Deceptively simple, but in fact nontrivial for homogenization.
- Precise definitions and TR results are seldom given. (Take volume averages and make sure the results are pleasing to the eye.)
- Only dispersion relations, but not the boundary conditions, are usually considered.

Vadim Markel and IT, Phys Rev B 88, 125131, 2013.
IT and Vadim Markel, Proc Royal Soc A, May 2014.
S. Tang, B. Zhu, M. Jia, Q. He, S. Sun, Y. Mei, and L. Zhou
Phys Rev B 91, 174201, 2015.

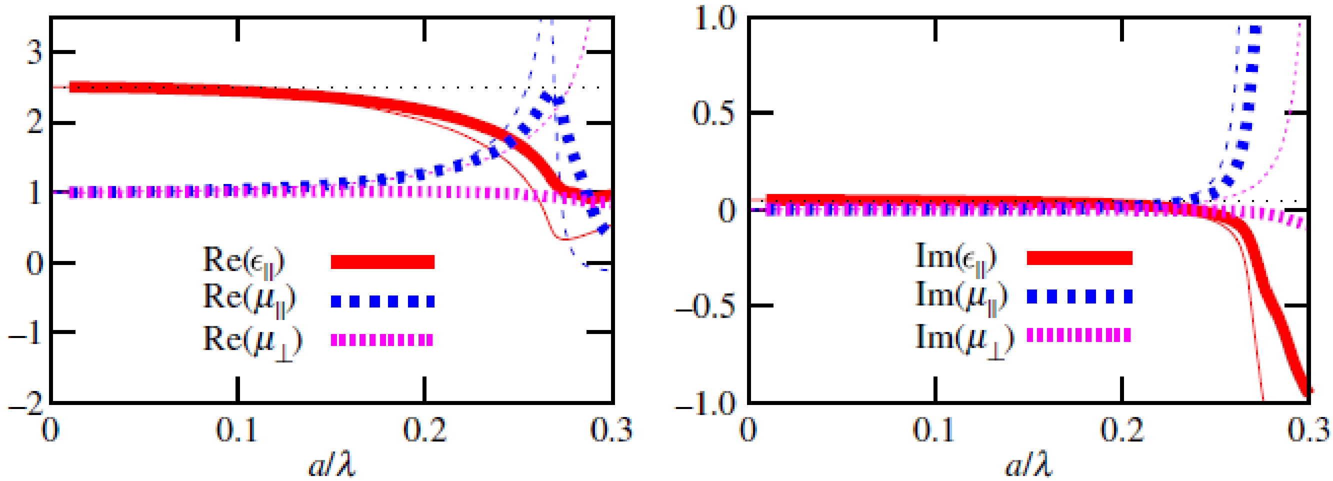
Numerical Example: Layered Medium

- Layered dielectric structure, *s*-mode.
- Analytical solution used for error analysis.
- $\varepsilon_a = 4.0 + 0.1i$
- $\varepsilon_b = 1$



Vadim Markel and IT, Phys Rev B 88, 125131 (2013).

Local Effective Parameters



Example 1. Effective parameters by Trefftz homogenization (thick lines) and by S-parameter retrieval (thin lines) as functions of a/λ; the lattice period a changes while λ is fixed. The dotted line represents the classical homogenization limit for $\epsilon_{\|}$ (in s-polarization, the volume average of ϵ_1 and ϵ_2).

Up to a/λ~0.15, the agreement between Trefftz homogenization and parameter retrieval is almost perfect but then they diverge. This is because Trefftz homogenization optimizes effective parameters in a wide range of propagation angles while S-parameter retrieval optimizes T/R only for near-normal incidence.

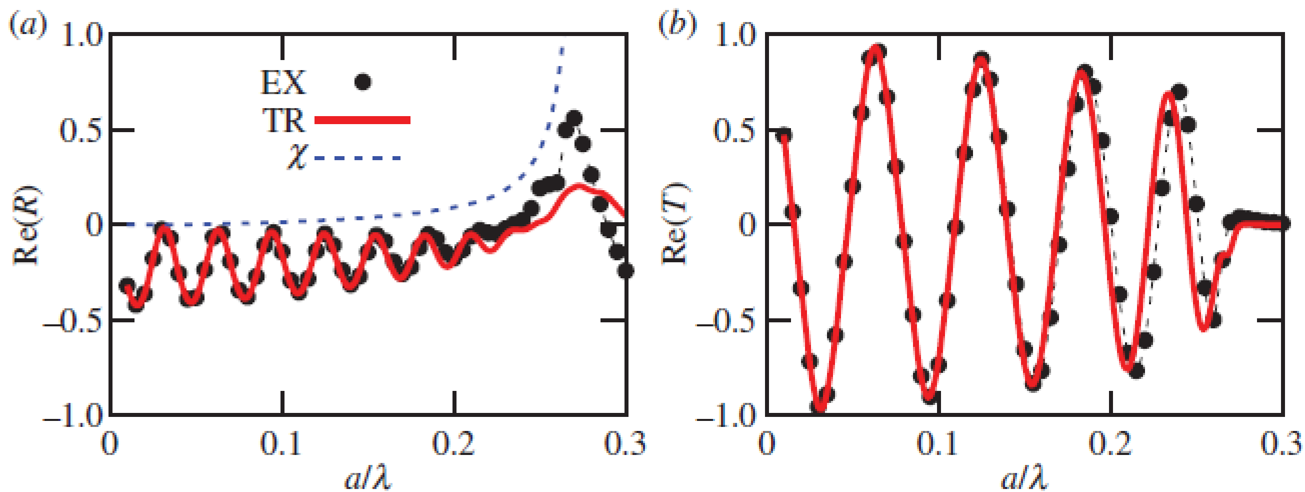
PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

A non-asymptotic homogenization theory for periodic electromagnetic structures

Igor Tsukerman and Vadim A. Markel

Proc. R. Soc. A 2014 **470**, 20140245, published 28 May 2014

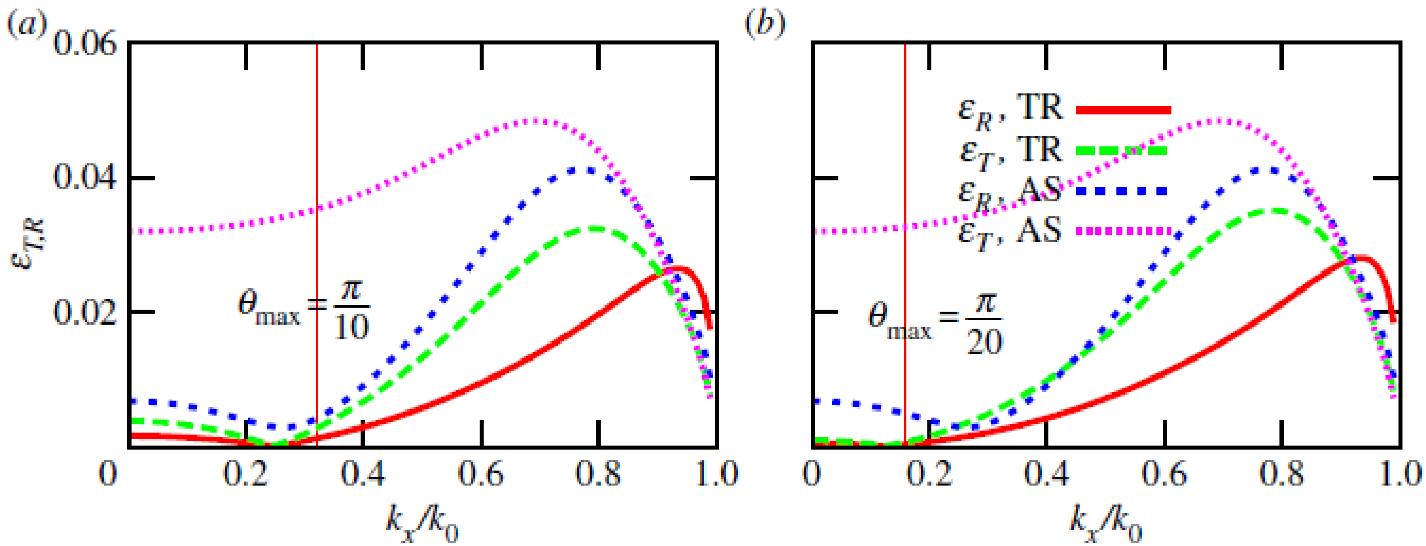
TR vs. a/λ (local homogenization)



Example 1. (*a*) Real parts of the reflection coefficient R and (*b*) transmission coefficient T, and the homogenization error indicator χ (4.2) (*a*) for the layered structure consisting of $L = 10$ elementary cells and for the equivalent homogenized slab as functions of a/λ. EX, exact results; TR, Trefftz homogenization.

R/T defined as the ratios of the complex amplitudes of the reflected/transmitted and incident tangential fields (the electric field for *s*-polarization). Normal incidence. Error indicator χ relatively small for $a/\lambda \leq 0.2$ but grows rapidly beyond that range. Hence homogenization is accurate for $a/\lambda \leq 0.2$ but otherwise the medium is not homogenizable (at least in terms of local parameters).

TR vs. angle (local homogenization)



Example 1. Errors in the transmission and reflection coefficients (5.1) as functions of the sine of the incidence angle, $\sin\theta = k_x/k_0$, for $a/\lambda = 0.2$. The errors are displayed for Trefftz homogenization (TR) and for the classical asymptotic homogenization limit (AS). The maximum angles of incidence in the restricted set of basis functions for Trefftz homogenization ((*a*) $\theta_{\max} = \pi/10$ and (*b*) $\theta_{\max} = \pi/20$) are indicated by the vertical lines.

One may wish to tailor the effective parameters to a restricted range of incidence angles. Trade-off between the range of applicability and accuracy of the effective medium description.

PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

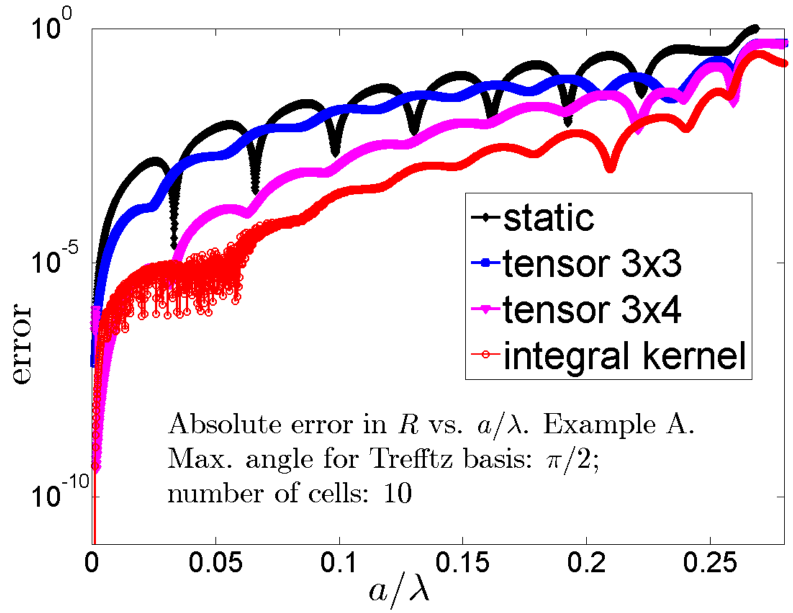
A non-asymptotic homogenization theory for periodic electromagnetic structures

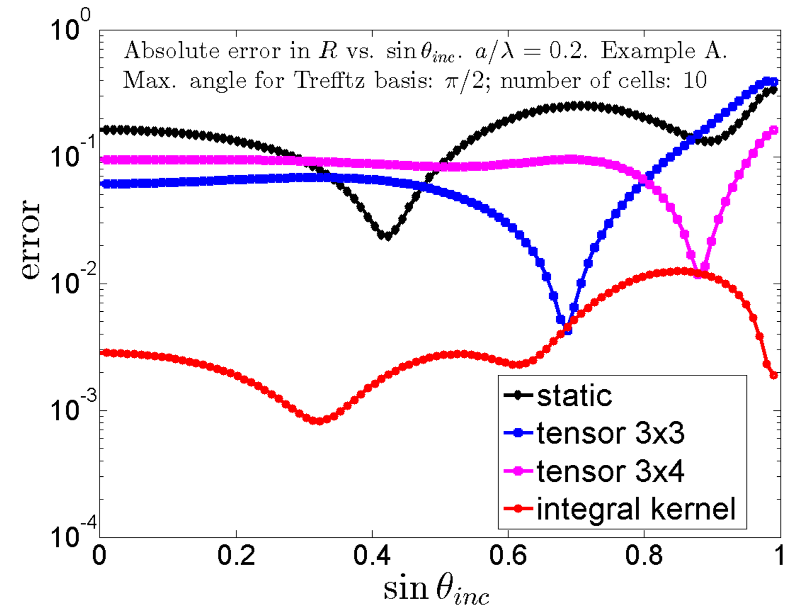
Igor Tsukerman and Vadim A. Markel

Proc. R. Soc. A 2014 **470**, 20140245, published 28 May 2014

Nonlocal Homogenization (work in progress)

$$\varepsilon_a = 4.0 + 0.1i$$
$$\varepsilon_b = 1$$

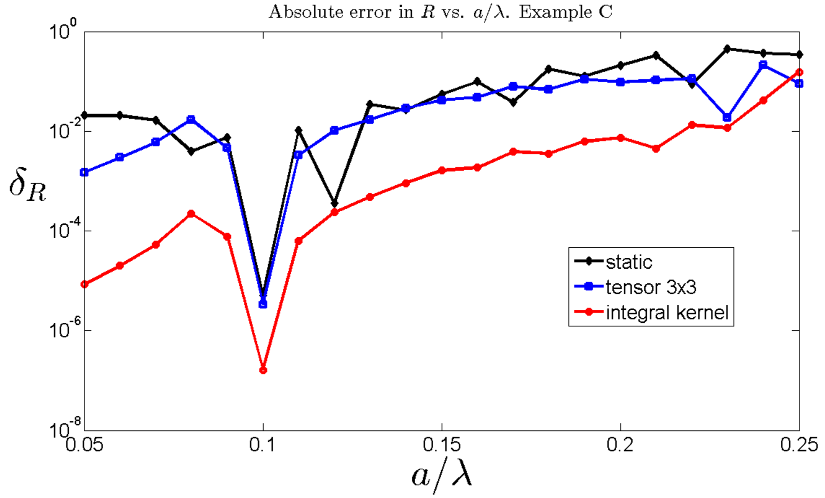


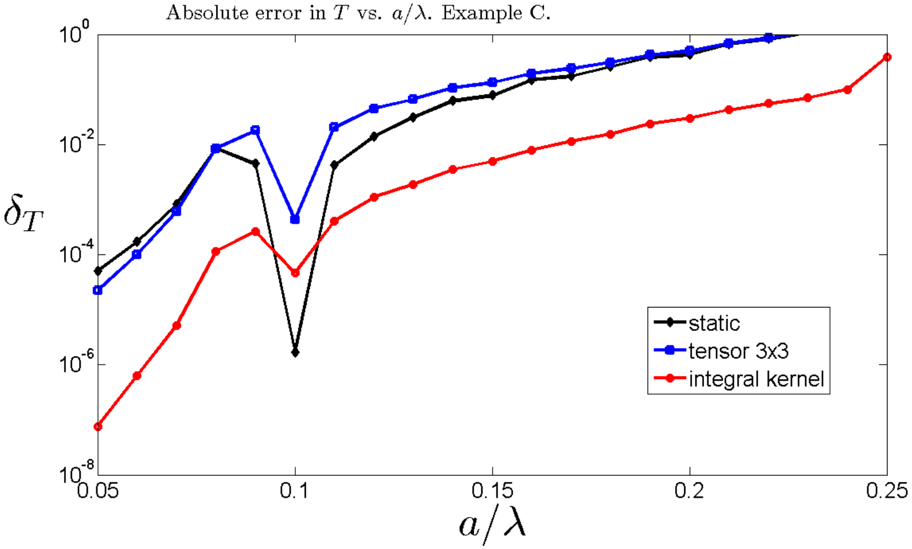


Errors in the reflection coefficient *R* vs. a/λ (left; first photonic band) and vs. sin θ (right). The nonlocal integral model (red line) is seen to be much more accurate than the static (asymptotic) tensor (black line) and than the local model (blue line)..

Nonlocal Homogenization (work in progress)

$$\epsilon_a = \epsilon_0 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$$





Same as before but for Example C of VM & IT, PRB 2013: Drude model for silver as material a; material b is air. $\varepsilon_0 = 5$, $\omega_p = 500\gamma$, $\lambda_p = 2\pi\omega_p / c \approx 136$nm, $a = 0.2\lambda_p \approx 27$ nm.

Conclusion

- Not only bulk relations but also boundary conditions are critical for homogenization.
- Nontrivial magnetic response of periodic structures composed of intrinsically nonmagnetic constituents has limitations and is subject to an “uncertainty principle”.
- Namely, the stronger the magnetic response, the less accurate (“certain") are predictions of the effective medium theory.

Conclusion (cont'd)

- In practice, there is still room for engineering design, but trade-offs between magnetic response and the accuracy of homogenization must be noted.
- Basis for analysis: coarse-level fields must satisfy the dispersion relation *and boundary conditions* accurately.
- Not only the dispersion relation but also surface impedance have to be illumination independent if homogenization were to be accurate.
- These prerequisites cannot unfortunately hold simultaneously if the desired magnetic response is strong.

Conclusion (cont'd)

- Instructive numerical example: triangular lattice of cylindrical air holes in a dielectric host (Pei & Huang). 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.
- Nonlocal homogenization may further improve the accuracy by about an order of magnitude.

The End