Meta-Materials for light: Homogenization of Maxwell equations

Workshop “Variational Views in Mechanics and Materials”

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Is $\frac{7}{6}$ a small number?
Strange behavior of light: Two examples
Perfect transmission through sub-wavelength structures
Negative index Materials

Shortest Paths

Fermat’s principle of the fastest path:
Light finds the fastest way to reach the destination,

\[
\frac{\sin \Theta_1}{\sin \Theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}
\]

Wave equation

Huygens’ principle of superpositions

Wave equation

\[ \partial_t^2 u = \Delta u \]

Numerical solution

Meta-Materials for light: Homogenization of Maxwell equations
Maxwell’s Equations

**Variables:**
- Electric field $E$
- Magnetic field $H$

**Simplification:**
- Time harmonic solutions
  $$H, E \sim e^{-i\omega t}$$

**Remarks:**
- Vacuum: $\mu = \varepsilon = 1$
- Material parameter
  $$\text{Im } \varepsilon \leftrightarrow \text{conductivity}$$

\[
\begin{align*}
\text{curl } E &= i\omega \mu H \\
\text{curl } H &= -i\omega \varepsilon E
\end{align*}
\]
**Negative index of refraction**

**Veselago (1968)**

Properties of materials with negative index, Maxwell equations

If \( n_1 > 0 \) and \( n_2 < 0 \), then light should be refracted “backward”.

**But … in Maxwell’s Equations**

- \( \Re \varepsilon < 0 \) possible
- \( \mu \) is always 1
- \( \Re \mu \varepsilon < 0 \): light can not travel in the medium

**Negative Index:** \( \varepsilon \) and \( \mu \) negative!

Solutions for positive and negative index

Computer graphics: Negative refraction
Experimental construction of Meta-Materials

- Pendry et al. (≈ 2000) suggest a split ring construction

A negative index meta-material

- Experiments confirm the negative index
**Transmission through sub-wavelength holes**

**Observation:** Light hits a metal layer with holes. Even though the holes have sub-wavelength dimensions, the light can exit at the other side.

**Surface plasmons: A mathematicians view**

We consider the Helmholtz equation \( \nabla \cdot (a(x) \nabla u(x)) = -k^2 u(x) \) or even

\[
\nabla \cdot (a(x) \nabla u(x)) = 0
\]

Let \( a \) be \(+1\) for \( x_1 > 0 \) and \(-1\) for \( x_1 < 0 \), \( \omega > 0 \) arbitrary

\[
\begin{array}{c|c}
 x_1 < 0 & x_1 > 0 \\
 a = -1 & a = +1 \\
 u(x_1, x_2) = \exp(\omega x_1) \sin(\omega x_2) & u(x_1, x_2) = \exp(-\omega x_1) \sin(\omega x_2)
\end{array}
\]

Then \( u \) is harmonic and
and \( a(x) \partial_{x_1} u(x) \) is continuous

Similarly, solutions of the Helmholtz equation can be obtained
\( \rightarrow \) we found a wave solution that localizes at the interface
**Time-harmonic Maxwell Equations**

Later, \( \eta > 0 \) stands for the size of the holes ... 

\[
\text{curl } E_\eta = i\omega \mu_0 H_\eta \\
\text{curl } H_\eta = -i\omega \varepsilon_\eta \varepsilon_0 E_\eta
\]

Wave number \( k \) and wavelength \( \lambda = \frac{2\pi}{k} \). Further assumptions:

- invariance in direction \( x_3 \)
- magnetic transverse polarization \( H = (0, 0, u) \)

2D Helmholtz equation for \( H_\eta = (0, 0, u_\eta) \) with \( u_\eta = u_\eta(x_1, x_2) \)

\[
\nabla \cdot \left( \frac{1}{\varepsilon_\eta} \nabla u_\eta \right) = -k^2 u_\eta.
\]

**Question:** What is the behavior of \( u_\eta \) in the limit \( \eta \to 0 \)?
Geometry and permittivity

The domain $\Omega$: Maxwell equations are solved
Rectangle $R$: The original shape of the metal
Union of small rectangles $\Sigma_{\eta}$: The metal part after cutting holes

$$\varepsilon_{\eta}(x) = \begin{cases} \frac{\varepsilon_r}{\eta^2} & \text{for } x \in \Sigma_{\eta} \\ 1 & \text{for } x \notin \Sigma_{\eta} \end{cases}$$

**Note:** $|\varepsilon_{\eta}|$ is huge in the metal part!
First thoughts on the system

With \( a_\eta = 1/\varepsilon_\eta \) (order \( \eta^2 \) in the metal) we must study

\[
\nabla \cdot (a_\eta \nabla u_\eta) + k^2 u_\eta = 0 .
\]

1. Outside the metal: \( a_\eta \equiv 1 \rightarrow \text{no oscillations} \rightarrow \nabla_y u = 0 \)

2. In the metal: \( a_\eta = \eta^2 \varepsilon_r^{-1} \rightarrow \nabla_y \cdot (\varepsilon_r^{-1} \nabla_y u) + k^2 u = 0 \)

With aperture \( \alpha \in (0, 1) \) and metal thickness \( 2\gamma = 1 - \alpha \):
Define \( \Psi : \mathbb{R} \to \mathbb{C} \) as the continuous, 1-periodic solution of

\[
\begin{align*}
\partial_z^2 \Psi(z) &= -k^2 \varepsilon_r \Psi(z) \quad \text{for } z \in (-\gamma, \gamma) \quad \text{(metal)} \\
\Psi(z) &= 1 \quad \text{for } z \in [-1/2, 1/2] \setminus (-\gamma, \gamma) \quad \text{(void)}
\end{align*}
\]

\( \Psi \) is given by

\[
\Psi(z) = \begin{cases} 
\frac{\cosh(k\sigma z)}{\cosh(k\sigma \gamma)} & \text{for } |z| \leq \gamma \\
1 & \text{for } \gamma < |z| \leq 1/2
\end{cases}
\]
Qualitative behavior of solutions

We expect (in the rectangle $R$):

$$u_\eta \approx U(x_1, x_2) \Psi(x_1/\eta)$$

In particular, in the single slit:

$$u_\eta \approx U(x_2)$$

Here: $\varepsilon_r < 0$ real

Equation in the single slit is (for some $\tau \in \mathbb{C}$)

$$\frac{\partial^2}{\partial x_2^2} U = -k^2 \tau^2 U$$

Qualitative Argument: The second derivative $\partial_{x_1}^2 u_\eta$ in the slit is proportional to the values at the metal interfaces.

- Solutions $U(x_2)$ are $\cos(\tau k x_2)$ and $\sin(\tau k x_2)$
- For height $h > 0$ in resonance with $\tau$: Upper and lower boundary coupled
The effective system

**Original system:** with $a_\eta = 1/\varepsilon_\eta$

$$\nabla \cdot (a_\eta \nabla u_\eta) + k^2 u_\eta = 0 \quad \text{in } \Omega$$

**Limit system:** (loosely stated)

$$\nabla \cdot (a_{\text{eff}} \nabla U) + k^2 \mu_{\text{eff}} U = 0 \quad \text{in } \Omega$$

$a_{\text{eff}} : \mathbb{R}^2 \to \mathbb{R}^{2 \times 2}$ and $\mu_{\text{eff}} : \mathbb{R}^2 \to \mathbb{C}$ are effective coefficients

- $a_{\text{eff}}(x) := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\mu_{\text{eff}}(x) := 1$ for $x \in \mathbb{R}^2 \setminus R$
- $a_{\text{eff}}(x) := \begin{pmatrix} 0 & 0 \\ 0 & \alpha \end{pmatrix}$ and $\mu_{\text{eff}}(x) := \beta$ for $x \in R$

$\alpha > 0$: aperture volume $=$ relative slit width

$$\beta := \int_{-1/2}^{1/2} \Psi(z) \, dz = \frac{2}{k\sigma} \frac{\sinh(k\sigma \gamma)}{\cosh(k\sigma \gamma)} + \alpha \in \mathbb{C}.$$
Theorem (Bouchitté and S., 2012)

Assume $\beta \neq 0$, $\varepsilon_r \neq 0$, $a_\eta := \varepsilon_\eta^{-1}$ (small in the metal). Consider

$$\nabla \cdot j_\eta = -k^2 u_\eta, \quad j_\eta = a_\eta \nabla u_\eta,$$

with limits $u_\eta \rightharpoonup u$ and $j_\eta \rightharpoonup j$ in $L^2(\Omega)$ for $\eta \to 0$. Set

$$U(x) := \begin{cases} 
    u(x) & \text{for } x \in \Omega \setminus R \\
    \beta^{-1} u(x) & \text{for } x \in R
\end{cases}$$

There holds $\partial_{x_2} U \in L^2_{loc}(\Omega)$ and

$$j = \begin{cases} 
    (\partial_{x_1} U, \partial_{x_2} U) & \text{in } \Omega \setminus \overline{R} \\
    (0, \alpha \partial_{x_2} U) & \text{in } R
\end{cases}$$

and

$$\nabla \cdot j = -k^2 u \text{ in } \Omega$$
Method of proof

1.) Two-scale convergence: \( u_\eta \rightarrow u_0(x_1, x_2, y_1) \) with \( (u_\eta \rightharpoonup u) \)

\[
u_0(x, y) = \begin{cases} 
  u(x) & \text{for } x \notin R \\
  \beta^{-1}u(x) \Psi(y_1) & \text{for } x \in R
\end{cases}
\]

2.) Two-scale convergence: \( j_\eta \rightarrow j_0(x, y) \) with \( (j_\eta \rightharpoonup j) \)

\[
 j_0(x, y) = \begin{cases} 
  j(x) & \text{for } x \notin R \\
  \alpha^{-1}j_2(x) e_2 1_{\{|y_1| > \gamma\}} & \text{for } x \in R
\end{cases}
\]

3.) The distributional derivatives of \( U \) satisfies \( \partial_{x_2} U \in L^2(\Omega) \).

Furthermore

\[
 j(x) = \begin{cases} 
  (\partial x_1 U(x), \partial x_2 U(x)) & \text{for } x \notin \overline{R} \\
  (0, \alpha \partial x_2 U(x)) & \text{for } x \in R
\end{cases}
\]

To show this relation: Consider only the void!
Transmission properties

Ansatz ($R \in \mathbb{C}$ for reflection, $T \in \mathbb{C}$ for transmission):

$$U(x_1, x_2) = \begin{cases} 
  e^{ik(sin(\theta)x_1-cos(\theta)x_2)} + Re^{ik(sin(\theta)x_1+cos(\theta)x_2)} & \text{for } x_2 > 0, \\
  (A_1 \cos(\tau k x_2) + A_2 \sin(\tau k x_2)) e^{ik(sin(\theta)x_1} & \text{for } 0 > x_2 > -h, \\
  Te^{ik(sin(\theta)x_1-cos(\theta)(x_2+h))} & \text{for } -h > x_2.
\end{cases}$$

$\tau := \sqrt{\beta/\alpha}$ reflects the equation $\partial_{x_2}^2 U = -k^2 \tau^2 U$ in the structure.

At the (horizontal) interfaces:

- continuity of $U$
- continuity of $j \cdot e_2$
Results on transmission properties

A calculation with the transfer matrix provides for \( T \in \mathbb{C} \)

\[
T = \left( \cos(\tau kh) - \frac{i}{2} \left[ \frac{\alpha \tau}{\cos(\theta)} + \frac{\cos(\theta)}{\alpha \tau} \right] \sin(\tau kh) \right)^{-1}
\]

Physical values taken from Qing and Lalanne in non-dimensional form \((h = 1)\):

<table>
<thead>
<tr>
<th>( \eta = 7/6 )</th>
<th>( \alpha = 1/7 )</th>
<th>( \gamma = 3/7 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda = 15/6 )</td>
<td>( k = 2\pi/\lambda \approx 2.51 )</td>
<td>( \varepsilon_{\eta} = (0.12 + 3.7i)^2 )</td>
</tr>
</tbody>
</table>

Explicit formulas for

\[
\beta = \beta(\sigma, k, \alpha) \\
\tau = \tau(\beta, \alpha) \\
T = T(\tau, k)
\]

Left: \( T = T(k) \) for normal incidence, \( \theta = 0 \).
Right: \( T = T(\theta) \) for wave-number \( k = 0.8 \).
Conclusions on transmission

- We analyze: metal with large permittivity ($\eta^{-2}$) and small holes ($\eta$)
- Effective system is Maxwell-type, permittivity in $x_1$-direction is $+\infty$
- Natural field is $U$, not $u$ (field outside the metal).
  **The field** $U$ satisfies the continuity condition!
- Effective equations show the astonishing transmission $T \approx 1$
Negative index Meta-Materials

▶ Bouchitté, G. and Schweizer, B., SIAM J. Mult. Mod. 2010

A negative index material in experiments ... and in mathematics

\((H_\eta, E_\eta)\) solves the Maxwell system with a radiation condition at \(\infty\).

\[
\begin{align*}
\text{curl } E_\eta &= i\omega H_\eta \\
\text{curl } H_\eta &= -i\omega \varepsilon_\eta E_\eta
\end{align*}
\]
Microscopic geometry

“Many rings with thin slits”

The material parameter is

\[ \varepsilon_\eta = \begin{cases} 
1 + i \frac{\kappa}{\eta^2} & \text{in the rings} \\
1 & \text{else} 
\end{cases} \]

The parameter \( \eta \) appears 3×:

1. thin rings / many rings
2. high conductivity
3. very thin slit
Homogenization

The aim is to replace the **complex structure** of *many* split rings with *high conductivity* by a **homogeneous Meta-material**.

The resulting equations are of the form

\[
\text{curl } E = i\omega \mu_{\text{eff}} H \\
\text{curl } H = -i\omega \varepsilon_{\text{eff}} E
\]

For appropriate parameters holds \( \text{Re}(\mu_{\text{eff}}) < 0 \).
Main result

Let \( \varepsilon_\eta \) be given with \( \varepsilon_\eta = 1 + i \frac{\kappa}{\eta^2} \) in the rings. Let \( (H_\eta, E_\eta) \) solve the Maxwell system with a radiation condition at \( \infty \).

\[
\begin{align*}
\text{curl } E_\eta &= i \omega H_\eta \\
\text{curl } H_\eta &= -i \omega \varepsilon_\eta E_\eta
\end{align*}
\]

Theorem (Bouchitté – S. 2010, Lamacz – S. 2013)

Let \( (H_\eta, E_\eta) \rightharpoonup (H, E) \) in \( L^2_{loc}(\mathbb{R}^3) \) for \( \eta \to 0 \). Then, for matrices \( \hat{M}_\lambda \) and \( \hat{N} \), the limit functions solve

\[
\begin{align*}
\text{curl } E &= i \omega H \\
\text{curl } (\hat{M}_\lambda H) &= -i \omega \hat{N} E.
\end{align*}
\]

There holds \( \hat{M}_\lambda = M_0 + \lambda(\omega, \kappa)m_0 e_3 \otimes e_3 \) in \( \Omega \), with

\[
\lambda(\omega, \kappa) = \frac{-\varepsilon_0 \mu_0 \omega^2 D_3(\omega, \kappa)}{\alpha(\pi \rho)^{-1} + \varepsilon_0 \mu_0 \omega^2 D_0(\omega, \kappa) - i \kappa^{-1}}.
\]

Interpretation: The physical field is \( \hat{H} = \hat{M}_\lambda H \) such that \( H = \mu^{\text{eff}} \hat{H} \).
Formally, 1D-rings

Thin rings:

\[ Y = (0, 1)^3 \]
\[ \Sigma = S^1 \subset Y \]
\[ \dim(\Sigma) = 1 \]

Shape of \( J \):

\[ j_\eta := \eta \varepsilon_\eta E_\eta \rightarrow J \]
\[ \text{supp } J \subset \Sigma \]
\[ \text{div } J = 0 \]
\[ \Rightarrow J = j \tau H^1[\Sigma]. \]

This determines the non-trivial part of the magnetic field.

\[ \text{curl } E_\eta = i \omega H_\eta \]
\[ \text{curl } H_\eta = -i \omega \varepsilon_\eta E_\eta \]

Shape of \( H \):

\[ \text{curl } H = J \]
Homogenization procedure

\[ \text{curl } E_\eta = i\omega H_\eta \]
\[ \text{curl } H_\eta = -i\omega \varepsilon_\eta E_\eta \]

Two-scale convergence: \( H_\eta(x) \to H_0(x, y) \) and \( E_\eta(x) \to E_0(x, y) \) in the sense of two-scale convergence (\( L^2 \) or measures)

Loose definition: In the single periodicity cell \( Y = [0, 1]^3 \) the solution looks like

\[ H_\eta(x) \sim H_0(x, y), \quad E_\eta(x) \sim E_0(x, y), \]

where \( y \in Y \) is the local position within the cell.

The limits \( H_0(x, .) \) and \( E_0(x, .) \) solve the Maxwell equations, for example

\[ \text{div}_y H_0(x, y) = 0 \text{ in } Y, \quad \text{curl}_y E_0(x, y) = 0 \text{ in } Y, \]
\[ \text{curl}_y H_0(x, y) = 0 \text{ in } Y \setminus \Sigma. \]
The current $J$

\[
\text{curl } E_\eta = i\omega H_\eta \\
\text{curl } H_\eta = -i\omega \varepsilon_\eta E_\eta
\]

We additionally consider the field

\[J_\eta := \eta \varepsilon_\eta E_\eta \rightarrow J_0(x,y).
\]

Then

\[
\text{div } J_\eta = 0 \text{ implies } \text{div}_y J_0(x,) = 0 \text{ in } Y \\
E_\eta \text{ bounded implies } J_0(x,) = 0 \text{ in } Y \setminus \Sigma \\
\eta \text{ curl } H_\eta = -i\omega J_\eta \text{ implies } \text{curl}_y H_0(x,) = -i\omega J_0(x,) \text{ in } Y.
\]
Outline of the homogenization proof

1. Introduce current \( J_\eta := \eta \varepsilon_\eta E_\eta \) and derive estimates

2. Consider two-scale limits \( H_0, E_0, J_0 \) and derive cell problems
   Difficulty: Slit vanishes

3. Analyze cell problems.
   Difficulty: construction of the special solution \( H^0 \) “pointing through the ring”

4. Write the two-scale limit as

   \[
   H_0(x, y) = j(x) H^0(y) + \sum_{k=1}^{3} H_k(x) H^k(y),
   \]

   and determine \( j \) from the slit

5. Conclude the macroscopic equation

Result of 4: \( j(x) = \lambda H_3(x) \) with

\[
\lambda(\omega, \kappa) = \frac{-\varepsilon_0 \mu_0 \omega^2 D_3(\omega, \kappa)}{\alpha(\pi \rho)^{-1} + \varepsilon_0 \mu_0 \omega^2 D_0(\omega, \kappa)} - i\kappa^{-1}.
\]
Step 3: 3D-cell problem without slit

We must study the 3D cell problem:

The $H$-problem

$$\text{curl}_Y H + i\omega\varepsilon_0 J = 0 \text{ in } Y,$$

$$\text{div}_Y H = 0 \text{ in } Y,$$

$H$ is periodic in $Y$,

is coupled to the $J$-problem

$$\text{curl}_Y J + \kappa\omega\mu_0 H = 0 \text{ in } \Sigma,$$

$$\text{div}_Y J = 0 \text{ in } Y,$$

$J = 0 \text{ in } Y \setminus \bar{\Sigma}.$

Lemma (Bouchitté – S., 2010)

The solution space to the above problem is four-dimensional.
**Idea for the Lemma**

Space for solutions:

\[ X_0 := \left\{ u \in L^2_{per}(Y) : \text{div} \, u \in L^2(Y), \text{curl} \, u = 0 \text{ on } Y \setminus \Sigma \right\} \]

Bilinear form:

\[ b_0(u, v) := \int_Y \text{div} \, u \, \text{div} \, \bar{v} - i k_0^2 \int_Y u \, \bar{v} \]

**Regarding normalization:**

On the 3D-torus \( \Sigma \subset \mathbb{R}^3 \) exists a vector field \( \chi_a \) such that with

\[ \text{curl} \chi_a = 0, \quad \nabla \Phi : \chi_a = \nabla \Phi. \]

Normalize special solution \( u \) with

\[ \int_Y u \cdot e_k = 0 \text{ for } k = 1, 2, 3, \text{ and } \int_\Sigma u \cdot \chi_a = 1. \]
Step 4: Slit analysis

The flux $J_\eta$ is almost constant — across the slit!
(despite $\varepsilon_\eta = 1 + i\frac{\kappa}{\eta^2}$ in the ring)

\[ E_\eta \sim \begin{cases} \frac{1}{i\omega} \frac{1}{\eta} j_0 \tau & \text{in the slit} \\ \frac{-1}{\kappa \omega} \eta j_0 \tau & \text{inside the material} \end{cases} \]

\[ \int_{\text{closed ring}} E_\eta \cdot \tau = \int_{\text{disc}} e_3 \cdot \text{curl} \ E_\eta = i\omega \int_{\text{disc}} e_3 \cdot H_\eta \]

... and in the limit $\eta \to 0$:

\[ -\frac{2i}{\omega} \left( \alpha - i\frac{\beta \pi}{\kappa} \right) j_0(x) = i\omega (D_3 H_3(x) - D_0 j_0(x)) \]

This provides $j_0(x) = \lambda(\omega) H_3(x)$. 
Step 5: Macroscopic equation

Use test-functions $\Phi$ from $\Phi(x, y) = \psi(x)\Theta(y)$ with $\text{curl}_y \Theta = 0$ in $Y$, $\Theta \equiv 0$ on $\text{conv } \Sigma$. Then, for $\eta \to 0$,

$$
\int_{\mathbb{R}^3} \text{curl } H_\eta \cdot \Phi = \int_{\mathbb{R}^3} (-i\omega \varepsilon_\eta E_\eta) \cdot \Phi \to \langle -i\omega E(x), \psi(x) \rangle
$$

... and the left hand side equals

$$
\int_{\mathbb{R}^3} H_\eta \cdot \text{curl } \Phi = \int_{\mathbb{R}^3} H_\eta(x)\Theta(x/\eta) \wedge \nabla \psi(x) \, dx
$$

$$
\to \int_{\mathbb{R}^3} \int_Y \{ H(x) + \lambda(\omega) H_3(x) H^0(y) \} \Theta(y) \wedge \nabla \psi(x) \, dy \, dx
$$

$$
= \int_{\mathbb{R}^3} [\hat{M} H(x)] \wedge \nabla \psi(x) \, dx = \langle \text{curl } [\hat{M} H], \psi(x) \rangle
$$

This provides $\text{curl } [\hat{M} H] = -i\omega E(x)$. 

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Conclusions on negative index materials

- split ring geometry with highly conducting rings
- 3D-scattering problem, Maxwell equations
- formulas for $\mu_{\text{eff}}$ and $\varepsilon_{\text{eff}}$ in terms of conductivity and geometric quantities
- mathematical proofs for the homogenization result
- Calculations show: $\mu_{\text{eff}}$ can be negative (despite $\mu_0 \equiv 1$)

Thank you!
All formulas (perfect transmission):

Permittivity with $\sigma^2 = -\varepsilon_r$

$$
\varepsilon_\eta(x) = \begin{cases} 
\frac{\varepsilon_r}{\eta^2} & \text{for } x \in \Sigma_\eta \\
1 & \text{for } x \notin \Sigma_\eta
\end{cases}
$$

Use $a_\eta = 1/\varepsilon_\eta$

$$
\beta = \frac{2}{k\sigma} \frac{\sinh(k\sigma\gamma)}{\cosh(k\sigma\gamma)} + \alpha \\
\tau = \sqrt{\frac{\beta}{\alpha}} \\
T = \left( \cos(\tau kh) - \frac{i}{2} \left[ \frac{\alpha\tau}{\cos(\theta)} + \frac{\cos(\theta)}{\alpha\tau} \right] \sin(\tau kh) \right)^{-1}
$$