Homogenization of Structured Materials

Mário G. Silveirinha
Why “homogenization”?

- Homogenization may enable a simplified description of very complex systems formed by many atoms (in case of natural media) or inclusions (in case of structured materials).

Liu et al., Nature Materials, DOI: 10.1038/nmat2072
Basic notions:

• Let $F$ be some physical entity. The macroscopic (spatially averaged) $\langle F \rangle$ is defined as,

\[
\langle F \rangle (r) = \int F(r - r') f(r') \, d^3r'
\]

where $f$ is a test function.
Example (1D):

Test function:

\[ f(x) = \begin{cases} 
1/D & \text{if } |x| < D/2 \\
0 & \text{otherwise}
\end{cases} \]
Properties of the test function:

- Real valued.
- Nonzero in some neighbourhood of the origin.
- Integral over all space is unity: \( \int f(\mathbf{r}) d^3\mathbf{r} \)
- The support of the test function must be greater than the characteristic dimension of the inclusions, and much smaller than the wavelength.

Example:

\[
 f(\mathbf{r}) = (\pi R^2)^{-3/2} e^{-r^2/R^2}
\]
A different perspective of spatial averaging:

\[
\langle F \rangle (\mathbf{r}) = \int F(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') \, d^3 \mathbf{r}'
\]

convolution

The test function \( f \) may be regarded as the “impulse response” of a linear system. Thus, the spatial averaging operation may be regarded as filtering.
Different perspective of spatial averaging (contd.)

\[
\langle F \rangle (r) = \frac{1}{(2\pi)^3} \int \tilde{f}(k) \tilde{F}(k) e^{-jkr} d^3k \\
\text{where} \quad \tilde{f}(k) = \int f(r) e^{+jkr} d^3r
\]

Since the spatial average procedure may be regarded as low pass filtering, we may choose \( f \) as an ideal low pass filter:

\[
\tilde{f}(k) = \begin{cases} 
1, & k \in B.Z. \\
0, & \text{otherwise}
\end{cases}
\]

Later, we will see that this can be useful...
“Microscopic” Maxwell’s Equations

\[ \nabla \times \mathbf{E} = -j \omega \mathbf{B} \]

\[ \nabla \times \left( \frac{\mathbf{B}}{\mu_0} \right) = \mathbf{J}_e + \varepsilon_0 \varepsilon_r j \omega \mathbf{E} \]

\( \mathbf{E} \) and \( \mathbf{B} \) – “microscopic” electric and induction fields

\( \mathbf{J}_e \) – microscopic external density of current

\( \varepsilon_r \) relative permittivity of the structured material
Homogenized Maxwell’s Equations

\[
\langle E \rangle(r) = \int E(r-r') f(r') d^3r' \\
\downarrow \\
\nabla \times \langle E \rangle(r) = \int \nabla \times E(r-r') f(r') d^3r' = \langle \nabla \times E \rangle(r)
\]

\[
\nabla \times \langle E \rangle(r) = \langle \nabla \times E \rangle(r)
\]

The spatial derivatives commute with the averaging operator!

Thus, the structure of Maxwell’s equations is preserved by the homogenization process.
Homogenized Maxwell’s Equations (contd.)

\[ \nabla \times \langle \mathbf{E} \rangle = -j\omega \langle \mathbf{B} \rangle \]

\[ \nabla \times \frac{\langle \mathbf{B} \rangle}{\mu_0} = \langle \mathbf{J}_e \rangle + \langle \mathbf{J}_d \rangle + j\omega\varepsilon_0 \langle \mathbf{E} \rangle \]

\[ \mathbf{J}_d = \varepsilon_0 (\varepsilon_r - 1) j\omega \mathbf{E} \] – induced “microscopic” current relative to the host medium

The key problem in homogenization theory:

How to relate \( \langle \mathbf{J}_d \rangle \) with the macroscopic fields \( \langle \mathbf{E} \rangle \) and \( \langle \mathbf{B} \rangle \)?
Physical insights into

\[ \langle J_d \rangle = \int f(\mathbf{r}') J_d(\mathbf{r} - \mathbf{r}') d^3\mathbf{r}' \]

Small dielectric scatterer:

The microscopic density of current induced in a small scatterer may be approximated by:

\[ J_d(\mathbf{r}) \approx j\omega p_e \delta(\mathbf{r}) + \nabla \times \left\{ \frac{p_m}{\mu_0} \delta(\mathbf{r}) \right\}. \]

- \( p_e \) – electric dipole moment
- \( p_m \) – magnetic dipole moment

Thus, for a collection of obstacles we have that:

\[ \langle J_d \rangle \approx j\omega \mathbf{P} + \nabla \times \mathbf{M} + \ldots \]
Classical Constitutive Relations
Macrosopic Electromagnetism

“Classical” theory is based on the decomposition:

\[ \langle J_d \rangle \approx j\omega P + \nabla \times M + \ldots \]

Spatial average of the microscopic currents

\[ \begin{align*}
    \nabla \times \langle E \rangle & = -j\omega \langle B \rangle \\
    \nabla \times \frac{\langle B \rangle}{\mu_0} & = \langle J_e \rangle + \langle J_d \rangle - j\omega\varepsilon_0 \langle E \rangle
\end{align*} \]

\[ \begin{align*}
    D & = \varepsilon_0 \langle E \rangle + P \\
    H & = \frac{\langle B \rangle}{\mu_0} - M
\end{align*} \]

\[ \begin{align*}
    \nabla \times \langle E \rangle & = -j\omega \langle B \rangle \\
    \nabla \times H & = \langle J_e \rangle + j\omega D
\end{align*} \]
Local Linear Media

For local linear (bianisotropic) media:

\[
\begin{align*}
D &= \varepsilon_0 \varepsilon_r \langle E \rangle + \sqrt{\varepsilon_0 \mu_0} \xi \cdot H \\
\langle B \rangle &= \sqrt{\varepsilon_0 \mu_0} \zeta \cdot \langle E \rangle + \mu_0 \mu_r \cdot H
\end{align*}
\]

\(\varepsilon_r (\omega)\) is the relative permittivity, \(\mu_r (\omega)\) is the relative permeability. 

\(\xi (\omega)\) and \(\zeta (\omega)\) are (dimensionless) parameters that characterize the magnetic-electric coupling.
Some problems with the application of classical homogenization theories to metamaterials:

• The characteristic dimensions of most metamaterials is about one tenth of the wavelength. And this is not only because of fabrication limitations…

Example: Split Ring Resonators!
To get a strong magnetic response the perimeter of the rings must be comparable to $\lambda/2$.

(Other options at microwaves: use lumped elements, distance between rings very small, rings printed on high dielectric substrates).

This is understandable... we are trying to obtain a material with a magnetic response from a metal which is a material with completely different properties ($\varepsilon=\infty$).
Some problems with the application of classical homogenization theories to metamaterials (contd.)

• The relatively large electrical size of the inclusions implies that higher-order multipoles (quadrupole moment, etc) may not be negligible…

\[
\langle J_d \rangle = j \omega P + \nabla \times M + \text{higher order multipoles}
\]

• It may not be possible to relate the electric field with the polarization vector through local relations, i.e. the material response may be nonlocal.

The homogenization of metamaterials may thus require more sophisticated and complex methods that can take into account and describe these phenomena.
Spatial Dispersion
Why time dispersion?

The electric charges cannot respond instantaneously to an applied electric field.
(For harmonic excitation, the electric dipole moment becomes out of phase with the applied electric field.)
Spatial dispersion emerges when the response of the basic inclusions does not depend uniquely on the behaviour of the fields in a small neighbourhood.

In other words, the electromagnetic fields at a given point of space may influence significantly the response of an inclusion situated at a significant distance from that point (larger than the characteristic microscopic dimension of the material).
Spatial dispersion (contd.)

Local material:

\[ p_e(0) = p_e(\langle E \rangle(0)) \]

Nonlocal material:

\[ p_e(0) = p_e(\langle E \rangle_{\text{all space}}) = p_e(\langle E \rangle(0), \langle E \rangle(r_1), \langle E \rangle(r_2), \ldots) \]
Understanding spatial dispersion

The wire medium has strong spatial dispersion even for extremely large wavelengths.
The electric current along the wire depends on the electric field along the whole axis, and not only on what happens in some neighbourhood.

\[ p_e = \frac{1}{j\omega} \frac{I}{A_{cell}} \]

The flow of electric charges may be regarded as a slow diffusion process which originates the nonlocal response.
Constitutive relations for spatially dispersive media
Some preliminary considerations

For spatially dispersive materials the decomposition of the average microscopic current into mean and eddy currents is not meaningful.

\[ \langle J_d \rangle = j\omega P + \nabla \times M + \ldots \] (not interesting)

The problem is that \( P \) and \( M \) cannot be related with the macroscopic fields through local relations.

Besides that, the higher-order multipoles may not be negligible.
Constitutive relations

\[
\begin{align*}
D_g &= \varepsilon_0 \langle E \rangle + P_g \\
H_g &= \frac{\langle B \rangle}{\mu_0}
\end{align*}
\]

\[
\nabla \times \langle E \rangle = -j\omega \langle B \rangle
\]

\[
\nabla \times \frac{\langle B \rangle}{\mu_0} = \langle J_e \rangle + \langle J_d \rangle + j\omega\varepsilon_0 \langle E \rangle
\]

\[
\nabla \times H_g = \langle J_e \rangle + j\omega D_g
\]

\[
P_g = \langle J_d \rangle / j\omega
\]

\[
= P + \nabla \times M / j\omega
\]

The effect of both the electric and magnetic dipole moments (as well as the effect of all other multipoles) is described by the (generalized) electric displacement vector.
Constitutive relations in periodic linear media:

\[
P_g(r) = \varepsilon_0 \int \chi_e (r - r') \cdot \langle E(r') \rangle \, d^3 r'
\]

\[
D_g(r) = \int \hat{\varepsilon}(\omega, r - r') \cdot \langle E(r') \rangle \, d^3 r'
\]

Dielectric function

In spatially dispersive media all the effects can be described solely by a dielectric function, being unnecessary to introduce a magnetic permeability, and/or magnetoelectric tensors.
Constitutive relations in the spectral domain:

The Fourier transform of the macroscopic electric field is:

\[ \langle \tilde{E} (k) \rangle = \int \langle E (r) \rangle e^{jk \cdot r} \, d^3 r \]

where \( k = (k_x, k_y, k_z) \)

In the spectral domain the constitutive relations become:

\[ \vec{D}_g \equiv \varepsilon_0 \langle \tilde{E} \rangle + \vec{P}_g = \varepsilon (\omega, k) \cdot \langle \tilde{E} \rangle \]

\[ \vec{H}_g = \frac{\langle \tilde{B} \rangle}{\mu_0} \]

\[ \varepsilon (\omega, k) = \int \hat{\varepsilon}(r, k) e^{jk \cdot r} \, d^3 r \]
Macrossopic Maxwell’s Equations in the Spectral domain:

\[ \mathbf{k} \times \langle \tilde{\mathbf{E}} \rangle = \omega \mu_0 \tilde{\mathbf{H}}_g \]

\[ -\mathbf{k} \times \tilde{\mathbf{H}}_g = -j \langle \tilde{\mathbf{J}}_e \rangle + \omega \varepsilon(\omega, \mathbf{k}) \langle \tilde{\mathbf{E}} \rangle \]

Important remark:

• Both \( \omega \) and \( k \) are independent variables of the dielectric function. This should be very clear from the definition.

• Sometimes this is a source of confusion, because for plane waves \( \omega \) and \( k \) are related by a relation of the type \( \omega = \omega(k) \).
Calculation of the Dielectric Function
How can we compute the dielectric function of a periodic structured material?

\[
\frac{k}{\omega} \times \langle \vec{E} \rangle = \langle \vec{B} \rangle \\
- \frac{k}{\omega} \frac{\langle \vec{B} \rangle}{\mu_0} = \frac{1}{j\omega} \langle \vec{J}_e \rangle + \varepsilon(\omega, k) \cdot \langle \vec{E} \rangle
\]

This should be valid for every external applied current.

Unit cell:
Remember the definitions:

\[ \mathbf{E} \text{ and } \mathbf{B} \text{ – “microscopic” electric and induction fields} \]

\[ J_e \text{ – microscopic external density of current} \]

\[ \langle \mathbf{E}(r) \rangle = \int \mathbf{E}(r - r') f(r') d^3r' \]

\[ \langle \mathbf{E}(\mathbf{k}) \rangle = \int \langle \mathbf{E}(\mathbf{r}) \rangle e^{i \mathbf{k} \cdot \mathbf{r}} d^3 \mathbf{r} \]

Thus,

\[ \langle \mathbf{\tilde{E}}(\mathbf{k}) \rangle = \mathbf{\tilde{E}}(\mathbf{k}) \tilde{f}(\mathbf{k}) \]
Main idea:

To define the dielectric function so that the system,

\[ \frac{k}{\omega} \times \langle \vec{E} \rangle = \langle \vec{B} \rangle \]

\[ \frac{k}{\omega \mu_0} \times \frac{\langle \vec{B} \rangle}{\langle \vec{J}_e \rangle} = \frac{1}{j\omega} \langle \vec{J}_e \rangle + \varepsilon(\omega, k) \cdot \langle \vec{E} \rangle \]

is verified for a microscopic external current of the form:

\[ J_e = J_{e,av} e^{-jk.r} \]

for arbitrary constant vectors.
Characterization of the macroscopic fields for a microscopic current with the Floquet property:

Solution of the problem is of the form:

\[ E(r) = \sum J e^{-jk_J \cdot r}, \quad k_J = k + k^0_J \]

\[ E_J = \frac{1}{V_{\text{cell}}} \int_{\Omega} E(r) e^{jk_J \cdot r} d^3r \]

\[ k^0_J = j_1 b_1 + j_2 b_2 + j_3 b_3 \]
Characterization of the macroscopic fields for a microscopic current with the Floquet property (contd.):

\[ E(\mathbf{r}) = \sum_{J} E_{J} e^{-j k_{J} \cdot \mathbf{r}} \]

\[ \langle \tilde{E}(k') \rangle = (2\pi)^{3} \sum_{J} E_{J} \tilde{f}(k_{J}) \delta(k' - k_{J}) \]

Choosing the test function as an ideal low pass-filter

\[ \tilde{f}(k') = \begin{cases} 1, & k' \in \text{B.Z.} \\ 0, & \text{otherwise} \end{cases} \]

\[ \langle \tilde{E}(k') \rangle = (2\pi)^{3} E_{\text{av}} \delta(k' - k) \]

\[ E_{\text{av}} = \frac{1}{V_{\text{cell}}} \int_{\Omega} E(\mathbf{r}) e^{+j \mathbf{k} \cdot \mathbf{r}} d^{3} \mathbf{r} \]

\[ \langle E \rangle = E_{\text{av}} e^{-j \mathbf{k} \cdot \mathbf{r}} \]
Characterization of the macroscopic fields for a microscopic current with the Floquet property (contd.):

Thus, we conclude that for electromagnetic fields with the Floquet property the macroscopic fields may be identified with the zero-order Floquet harmonics:

\[ \langle E \rangle = E_{av} e^{-jkr} \]

\[ \langle B \rangle = B_{av} e^{-jkr} \]

\[ D_g = (\varepsilon_0 E_{av} + P_{g,av}) e^{-jkr} \]

\[ = \varepsilon(\omega, k) E_{av} e^{-jkr} \]

\[ \langle J_e \rangle = j\omega P_{e,av} e^{-jkr} \]

\[ E_{av} = \frac{1}{V_{cell}} \int_{\Omega} E(r) e^{jk'r} d^3r \]

\[ B_{av} = \frac{1}{V_{cell}} \int_{\Omega} B(r) e^{jk'r} d^3r \]

\[ P_{g,av} = \frac{1}{V_{cell}} \int_{\Omega} J_d e^{jk'r} d^3r \]

\[ P_{e,av} = \frac{1}{V_{cell}} \int_{\Omega} J_e e^{jk'r} d^3r \]
Microscopic theory

The previous analysis implies that for an external source associated with a phase-shift defined by \( k \), the dielectric function should be defined consistently with the relation:

\[
\varepsilon(\omega, k) \cdot E_{\text{av}} = \varepsilon_0 E_{\text{av}} + P_{g,\text{av}}
\]

Unit cell:

\[
\begin{align*}
J_e &= J_{e,\text{av}} e^{-jk \cdot r} \\
P_{g,\text{av}} &= \frac{1}{V_{\text{cell}} j \omega \Omega} \int J_d e^{+jk \cdot r} d^3 r
\end{align*}
\]
Procedure to compute the dielectric function

The applied current is taken equal to: \( J_e = J_{e,av}e^{-jkr} \)

- For each \( \omega \) and \( k \), the microscopic Maxwell-Equations are solved for \( J_{e,av} \).

- With the computed microscopic fields we calculate:
  \[
  E_{av} = \frac{1}{V_{cell}} \int_{\Omega} E(r)e^{jkr} d^3r
  \]
  \[
  P_{g,av} = \frac{1}{V_{cell} j\omega} \int_{\Omega} J_d e^{jkr} d^3r
  \]

- Finally, using the obtained results \( (i=1,2,3) \) the dielectric function is obtained by imposing that: \( \varepsilon(\omega,k)E_{av} = \varepsilon_0 E_{av} + P_{g,av} \)
Some remarks

• **The homogenization problem is a source driven problem! It is not an eigenvalue problem.**

• **The computational domain may be taken equal to the unit cell.**
Plane wave solutions

\[-k \times E_{av} + \omega B_{av} = 0\]
\[\omega \varepsilon . E_{av} + k \times \frac{B_{av}}{\mu_0} = 0\]
\[\left( \left( \frac{\omega}{c} \right)^2 \frac{\varepsilon}{\varepsilon_0} + kk - k^2 I \right) \cdot E_{av} = 0\]

\[-1 - k \cdot \left( \left( \frac{\omega}{c} \right)^2 \frac{\varepsilon}{\varepsilon_0} - k^2 I \right)^{-1} \cdot k\]
\[E_{av} \propto \left( \frac{\varepsilon}{\varepsilon_0} - \frac{c^2 k^2}{\omega^2 I} \right)^{-1} \cdot \frac{c k}{\omega}\]

There is a one to one relation between plane waves in the homogenized medium and the Floquet eigenmodes of the structured material.
Homogenization of a lattice of electric dipoles
Periodic lattice of electric dipoles

Microscopic model:

\[ \frac{P_e}{\varepsilon_0} = \alpha_e(\omega) \cdot E_{loc} \]
The solution of the homogenization problem can be written in closed analytical form in terms of the lattice Green dyadic that verifies:

$$
G_p(r|r') = \left( I + \frac{\omega^2}{\omega c^2} \nabla \nabla \right) \Phi_p(r|r')
$$

$$
\nabla^2 \Phi_p + \left( \frac{\omega}{c} \right)^2 \Phi_p = -\sum I \delta (r - r' - r_t) e^{-jkr(\mathbf{r} - \mathbf{r'})}
$$
Microscopic electric field:

\[ E = (-j\omega\mu_0) G_p(r|0) \cdot j\omega P_e + (-j\omega\mu_0) V_{cell} G_{av} \cdot j\omega P_{e,av} e^{-jk \cdot r} \]

\[ G_{av} = \frac{1}{V_{cell}} \int_{\Omega} G_p(r|r') e^{+jk \cdot (r-r')} d^3r' \]

\[ G_{av} = \frac{1}{V_{cell}} \frac{1}{(\omega/c)^2} \frac{(\omega/c)^2 I - k k}{k^2 - (\omega/c)^2} \]

\[ G_{av}^{-1} = -V_{cell} \left[ ((\omega/c)^2 - k^2) I + k k \right] \]
The local field:

$$E_{loc} = \left(\frac{\omega}{c}\right)^2 \mathcal{G}_p' (0|0) \frac{P_e}{\varepsilon_0} + \left(\frac{\omega}{c}\right)^2 V_{cell} \mathcal{G}_{av} \frac{P_{e,av}}{\varepsilon_0}$$

Self contribution is removed

$$\mathcal{G}_p' (r|r') = \mathcal{G}_p (r|r') - \mathcal{G}_f (r|r')$$

The electric dipole moment of each particle can now be calculated using the microscopic equation:

$$\frac{P_e}{\varepsilon_0} = \alpha_e (\omega) \cdot E_{loc}$$
Generalized Lorentz-Lorenz formula:

\[ E_{loc} = \left( \frac{\omega}{c} \right)^2 G'_p (0|0) \cdot \frac{P_e}{\varepsilon_0} \left( \frac{\omega}{c} \right)^2 V_{cell} \frac{P_{e,av}}{\varepsilon_0} \]

Can be related with the macroscopic field

\[ E_{loc} = E_{av} + C_i (\omega, k) \cdot \frac{P_e}{\varepsilon_0} \]

\[ C_i (\omega, k) = \left( \frac{\omega}{c} \right)^2 \left( G'_p (0|0; \omega, k) - G_{av} (\omega, k) \right) \]

is the interaction dyadic
Generalized Lorentz-Lorenz formula (contd.):

\[ E_{loc} = E_{av} + C_i (\omega, k) \cdot \frac{P_e}{\varepsilon_0} \]

macroscopic field
The interaction dyadic:

\[
\begin{align*}
\bar{C}_{\text{int}}(r - r'; \omega, k) &= \left[ \left( \frac{\mu_s}{c} \right)^2 \mathbf{I} + \nabla \mathbf{v} \right] \Phi_{\text{reg}} \\
\Phi_{\text{reg}}(r, \omega, k) &= \frac{j \sin(\beta r)}{4\pi r} + \frac{1}{4\pi} \left[ \text{erfc}(Er) - 1 \right] \\
&\quad + \sum_{l \neq 0} \frac{1}{4\pi} \frac{\cos(\beta |r - r_l|)}{|r - r_l|} \text{erfc}(E|r - r_l|) e^{-j \mathbf{k} \cdot \mathbf{r}_l} \\
&\quad + \frac{1}{V_{\text{cell}}} \sum_{k = \pm} \frac{e^{-j \mathbf{k} \cdot \mathbf{r}}}{2k} \sum_{k = \pm} e^{-\left(k \pm \beta \right)^2/4E^2 - 1} \\
&\quad + \frac{1}{V_{\text{cell}}} \sum_{k \neq 0} \frac{1}{2|k_j|} \sum_{k_j = |k_j| + \beta} e^{-|k_j| \pm \beta \right)^2/4E^2} e^{-j \mathbf{k} \cdot \mathbf{r}}.
\end{align*}
\]
The interaction dyadic (contd.):

A classical result for highly symmetric lattices:

\[ C_i (\omega = 0, k = 0) = \frac{1}{3V_{\text{cell}}} I \quad (\text{s.c. lattice}) \]

The imaginary part of the interaction constant can be evaluated in closed analytical form:

\[ \text{Im} \{ C_i (\omega, k) \} = \frac{1}{6\pi} \left( \frac{\omega}{c} \right)^3 I \]
Calculation of the dielectric function:

\[ E_{\text{loc}} = E_{\text{av}} + C_i(\omega, k) \cdot \frac{P_e}{\varepsilon_0} \]

\[ \frac{P_e}{\varepsilon_0} = \alpha_e(\omega) \cdot E_{\text{loc}} \]

\[ P_{g,\text{av}} = \frac{P_e}{V_{\text{cell}}} \]

\[ (I - \alpha_e C_i) \cdot \frac{P_{g,\text{av}}}{\varepsilon_0} = \frac{1}{V_{\text{cell}}} \alpha_e E_{\text{av}} \]

\[ \varepsilon(\omega, k) = I + \frac{1}{V_{\text{cell}}} (I - \alpha_e C_i(\omega, k))^{-1} \cdot \alpha_e \]

**Generalized Clausius-Mossotti formula**
Some conclusions:

• The dielectric function of lattice of electric dipoles can be written in terms of an interaction dyadic and of the electric polarizability of an individual inclusion.

• The interaction constant may depend on the wave vector due to the intrinsic granularity of the material. This may result in strong spatial dispersion.

• It is possible to generalize the classical Lorentz-Lorenz and Clausius-Mossotti formulas to spatially dispersive materials.
Generalized Lorentz-Lorenz formulas for point particles with both electric and magnetic response:

\[ E_{\text{loc}} = E_{\text{ev}} + \bar{C}_{\text{int}}(\omega, k) \cdot \frac{P_e}{\varepsilon_0} + \bar{C}_{e,m}(\omega, k) \cdot c P_m. \]

\[ \frac{B_{\text{loc}}}{\mu_0} = H_{\text{av}} - \bar{C}_{e,\nu}(\omega, k) \cdot c P_e + \bar{C}_{\text{int}}(\omega, k) \cdot \frac{P_m}{\mu_0}. \]

\[ \bar{C}_{e,m}(\omega, k) = \frac{c}{j\omega} \nabla \times \bar{C}_{\text{int}}|_{r=0} = -j \frac{\omega}{c} \nabla \Phi_{\text{reg}}|_{r=0} \times \vec{l}. \]

More details in:


Generalized Lorentz-Lorenz formulas for microstructured materials

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(Received 20 August 2007; published 17 December 2007)

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Application of the results to a material formed by plasmonic spheres:

www.qcif.edu.au/research/Images/sc.gif

PHYSICAL REVIEW B 75, 024304 (2007)

Three-dimensional nanotransmission lines at optical frequencies: A recipe for broadband negative-refraction optical metamaterials

Andrea Alù and Nader Engheta
Homogenization model:

\[ \text{Re}\{\alpha_e^{-1}\} = \frac{(\varepsilon_r + 2)}{(\varepsilon_r - 1)3V_{\text{sph}}} \]

\[ V_{\text{sph}} = 4\pi R^3 / 3 \]

\[ \varepsilon_r = 1 - 3 \frac{\omega_r^2}{\omega^2} \]

For propagation along coordinate axes:

\[ \varepsilon_{\text{eff},xx} = 1 + \frac{1}{a^3} \frac{1}{\text{Re}\{\alpha_e^{-1}\}} - C_{xx}(\omega, k) \]

\[ C_{xx}(\omega, k) \approx \frac{1}{a^3} \left[ \frac{1}{3} - 0.15 \left( \frac{\omega}{c} \right)^2 - 0.026[\cos(k_x a) - 1] ight. 
- 0.026[\cos(k_y a) - 1] + 0.052[\cos(k_z a) - 1] \right] \]
Effective permittivity:

\[ R = \frac{\lambda}{100} \text{ at } \omega = \omega_r \]

\[ R = \frac{a}{2.1} \]
Band structure:

Backward wave propagation
Isofrequency contours:

Propagation in the xoy plane, with E along z. The contours specify the value of $\omega/\omega_c$. 

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Application of the results to a uniaxial material formed by SRRs

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May 5, Marrakech, 2008
"Classical model"

\[
\bar{\varepsilon} = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \bar{\mu} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mu \end{pmatrix}
\]

\[
\mu (\omega) = 1 + \left( \alpha^{-1} (\omega) - C \right)^{-1} / (a_x a^2)
\]

\[
\alpha = \left[ \left( \frac{\omega_r^2}{\omega^2} - 1 \right) \frac{L}{\mu_0 S^2} \right]^{-1}
\]

\[
C = \frac{\varepsilon_0 \pi R (\varphi - \pi)}{\cosh^{-1} \left( \frac{d^2}{2r^2} - 1 \right)}, \quad L = \mu_0 R \left[ \ln \left( \frac{8R}{r} \right) - 2 \right]
\]
Model obtained taking into account spatial dispersion

\[
\mu(\omega, k) = 1 + \left( \alpha^{-1}(\omega) - C(\omega, k) \right)^{-1} / (a_z a^2)
\]

\[
C(\omega, k) = \frac{1}{\pi R^2} \int_S C_{zz}^{zz} (r; \omega, k) \, ds
\]

Rings are modelled as particles with a dipole-type magnetic response.

**Note:** the effects of spatial dispersion could be described using uniquely a dielectric function. However, here we choose to define a spatially dispersive permeability to see better the connections with the classical model.
The interaction constant:

\[ C'(\omega, k) \approx \left[ C_0 + C_1 (\cos(k_z a_z) - 1) + C_2 \left( \frac{\omega a}{c} \right)^2 \right] \frac{1}{a^3} \]

\[ C_0 = 1.64 \quad C_1 = 0.43 \quad \text{and} \quad C_2 = -0.12. \]

Orthorhombic lattice with \( a_z = 0.5a \) and rings with \( R=0.4a \).
Effects of spatial dispersion:

Isofrequency contours

\[ r_w = 0.005a, \ d = 0.04a, \ \varphi = 350^\circ, \ R = 0.4a \ \text{and} \ a_z = 0.5a. \]
Regularized Formulation
A Mathematical Difficulty…

Microscopic Equations:

\[ \nabla \times \mathbf{E} = -j \omega \mathbf{B} \]

\[ \nabla \times \frac{\mathbf{B}}{\mu_0} = \mathbf{J}_{\text{e,av}} e^{-jk_r} + \varepsilon_0 j \omega \varepsilon_r \mathbf{E} \]

Applied current

Unit cell:

Problem:

If \((\omega,k)\) are associated with an electromagnetic mode the problem may not have a solution (a resonance is hit and the fields may grow without limit).
Relation between the applied current and the induced average electric field

It can be proven that the applied current is related to the induced microscopic and macroscopic electric field as follows:

\[ J_e = j\omega \left( \hat{P}_{av}(E_{av}) - \hat{P}(E) \right) e^{-jk.r} \]

where

\[ \frac{\hat{P}(E)}{\varepsilon_0} = \frac{1}{V_{cell}} \int_{\Omega} \left( \varepsilon_r - 1 \right) E e^{+jk.r} d^3r \]

\[ \frac{\hat{P}_{av}(E_{av})}{\varepsilon_0} = \frac{1}{\beta^2} \frac{1}{V_{cell}} G^{-1}_{av}.E_{av} \quad \text{with} \quad G^{-1}_{av} = -V_{cell} \left( \left( \beta^2 - k^2 \right) I + kk \right) \]
A mathematical trick:

**Microscopic Equations:**
\[ \nabla \times \mathbf{E} = -j \omega \mathbf{B} \]
\[ \nabla \times \frac{\mathbf{B}}{\mu_0} = J_{e,av} e^{-jk_r} + j \omega \varepsilon_0 \varepsilon_r \mathbf{E} \]

Source of fields is \( J_{e,av} \)

**Regularized microscopic equations:**
\[ \nabla \times \mathbf{E} = -j \omega \mathbf{B} \]
\[ \nabla \times \frac{\mathbf{B}}{\mu_0} = j \omega \left( \hat{P}_{e,av} (\mathbf{E}_{av}) - \hat{P} (\mathbf{E}) \right) e^{-jk_r} + \varepsilon_0 j \omega \varepsilon_0 \varepsilon_r \mathbf{E} \]

Source of fields is \( \mathbf{E}_{av} \)

**For corresponding \( J_{e,av} \) and \( \mathbf{E}_{av} \) the solution of the two problems is the same!**

However the kernel (null-space) of both problems is different. In fact, electromagnetic modes are not solutions of the homogeneous regularized problem.
Integral-differential system:

Regularized microscopic equations:

\[ \nabla \times \mathbf{E} = -j \omega \mathbf{B} \]
\[ \nabla \times \frac{\mathbf{B}}{\mu_0} = j \omega \left( \mathbf{P}_{av} - \mathbf{P} \right) e^{-jkr} + \varepsilon_0 j \omega \varepsilon \varepsilon_r \mathbf{E} \]

- For each \( \omega \) and \( k \), we solve the microscopic Maxwell-Equations with \( \mathbf{E}_{av} \square \hat{u}_i \)

- The dielectric function is obtained from:

\[ \mathbf{E} (\omega, k) \cdot \mathbf{E}_{av} = \varepsilon_0 \mathbf{E}_{av} + \mathbf{P}_{g,av} \]

\[ \mathbf{P}_{g,av} = \int_{\Omega} \mathbf{J} e^{-jkr} d^3 r \]

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Integral representation of the electric field:

\[
\mathbf{E}(\mathbf{r}) = \mathbf{E}_{av} e^{-j \mathbf{k} \cdot \mathbf{r}} + \int_{\partial D} \mathbf{G}_{p0}(\mathbf{r} | \mathbf{r}') \cdot \left( \mathbf{n}' \times \left[ \nabla' \times \mathbf{E} \right] \right) d\mathbf{s}' + \int_{\Omega - \partial D} \mathbf{G}_{p0}(\mathbf{r} | \mathbf{r}') \cdot \left( \frac{\omega}{c} \right)^2 (\varepsilon_r(\mathbf{r}') - 1) \mathbf{E}(\mathbf{r}') d^3\mathbf{r}'
\]

\[
\mathbf{G}_{p0} = \left( \mathbf{I} + \frac{c^2}{\omega^2} \nabla \nabla \right) \Phi_{p0}
\]

\[
\Phi_{p0}(\mathbf{r} | \mathbf{r}') = \Phi_{p}(\mathbf{r} | \mathbf{r}') - \frac{1}{V_{cell}} \frac{e^{-j \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}}{k^2 - \omega^2 / c^2}
\]
Solution based on the MoM:

\( \mathbf{w}_{n,k}(\mathbf{r}) \) - set of expansion functions for the induced microscopic current

\[
\frac{E_{\text{eff}}}{E_0}(\omega, \mathbf{k}) = \mathbf{I} + \frac{1}{V_{\text{cell}}} \sum_{m,n} \chi_{m,n} \int_{\Omega} \mathbf{w}_{m,k}(\mathbf{r}) e^{+j k \cdot \mathbf{r}} d^3 \mathbf{r} \otimes \int_{\Omega} \mathbf{w}_{n,-k}(\mathbf{r}) e^{-j k \cdot \mathbf{r}} d^3 \mathbf{r}
\]

\[
\chi_{m,n} = \int_{\Omega} \frac{1}{\varepsilon_r - 1} \mathbf{w}_{m,-k}(\mathbf{r}) \cdot \mathbf{w}_{n,k}(\mathbf{r}) d^3 \mathbf{r} - \int_{\Omega} \int_{\Omega} \mathbf{w}_{m,-k}(\mathbf{r}) \cdot \beta^2 \mathbf{G}_{p0}(\mathbf{r}|\mathbf{r}') \cdot \mathbf{w}_{n,k}(\mathbf{r}') d^3 \mathbf{r} d^3 \mathbf{r}'
\]

Green function
Application to wire media:

\[
\chi_{mn} = \int_D \int_D (\nabla_s w_{m,k}(r) \cdot \nabla' s w_{n,k}(r')) - \frac{\omega^2}{c^2} w_{m,k}(r) \cdot w_{n,k}(r') \Phi_{00}(r | r') ds ds'
\]

\[
\varepsilon_0 (\omega, k) = 1 + \frac{1}{V_{\text{cell}}} \sum_{m,n} \chi_{mn} \int_D w_{m,k}(r) e^{jkrds} \otimes \int_{s' D} w_{n,k}(r) e^{-jkrds}
\]
Application to wire media (contd.):

Within the thin wire approximation it may be assumed that the electric current flows along the direction of the wires and is uniform in the transverse section.

Thus a single expansion function may be sufficient to describe the electrodynamics of wire media.

\[ w_{1,k}(r) = \frac{e^{-jk_r}}{2\pi R} \hat{u}_z \]
The dielectric function:

\[
\frac{\varepsilon}{\varepsilon_0}(\omega, k) = \mathbf{I} + \frac{1}{V_{\text{cell}}} \frac{a^2}{\chi_{11}(\omega, k)} \hat{u}_z \hat{u}_z
\]

\[
\chi_{11}(\omega, k) = \left( k_z^2 - \frac{\omega^2}{c^2} \right) \frac{1}{(2\pi R)^2} \int_{\partial D} \int_{\partial D} \Phi_{p0}(r | r'; \omega, k) e^{ik \cdot (r-r')} ds ds'
\]

\[
\frac{\varepsilon}{\varepsilon_0}(\omega, k) = \mathbf{I} - \frac{\beta_p^2}{\omega^2/c^2 - k_z^2} \hat{u}_z \hat{u}_z
\]

\[
\frac{1}{\beta_p^2} = \frac{a}{(2\pi R)^2} \int_{\partial D} \int_{\partial D} \Phi_{p0}(r | r'; \omega, k) e^{ik \cdot (r-r')} ds ds'
\]
Similar ideas can be used to homogenize other materials:

\[
\varepsilon = \mathbf{I} - \frac{c^2 \beta_p^2}{\omega^2} \left( \mathbf{I} - \frac{kk}{k^2 - l_0 \omega^2 / c^2} \right)
\]
Similar ideas can be used to homogenize other materials (II):

$$\varepsilon = \left(1 - \frac{\beta_p^2}{\omega^2 / c^2 - k_x^2}\right) \hat{u}_x \hat{u}_x + \left(1 - \frac{\beta_p^2}{\omega^2 / c^2 - k_y^2}\right) \hat{u}_y \hat{u}_y + \left(1 - \frac{\beta_p^2}{\omega^2 / c^2 - k_z^2}\right) \hat{u}_z \hat{u}_z$$

Non-Connected WM
Similar ideas can be used to homogenize other materials (III):

Array of helices:

\[
\frac{\varepsilon_{\text{eff}}}{\varepsilon_0} = \begin{pmatrix}
\frac{A^2 k_x^2}{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2} & \frac{A^2 k_x k_y}{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2} & \frac{j A k_y}{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2} \\
\frac{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2}{A^2 k_x k_y} & \frac{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2}{A^2 k_y^2} & \frac{j A k_x}{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2} \\
\frac{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2}{A^2 k_x k_y} & \frac{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2}{A^2 k_y^2} & 1 - \frac{1}{\beta^2/\beta_{p1}^2 - k_x^2/\beta_{p2}^2}
\end{pmatrix}
\]
Extraction of the local parameters from the nonlocal dielectric function
Is it possible to extract local parameters from the nonlocal dielectric function?

Why local parameters?

- *The number of parameters that characterize the material is smaller.*

**Nonlocal model**

\[ \tilde{\varepsilon}(\omega, k) \]

Defined for every \( k \)

**Local model**

\[ \varepsilon_r(\omega), \mu_r(\omega), \xi(\omega), \zeta(\omega) \]

Independent of \( k \)
Is it possible to extract local parameters from the nonlocal dielectric function? (contd.)

Why local parameters?

- **Problems involving interfaces! The classical boundary conditions can only be applied to local media.**
Relation between local and nonlocal parameters

For a nonlocal medium:

\[ \varepsilon(\omega, k) \langle \vec{E} \rangle = \varepsilon_0 \langle \vec{E} \rangle + \vec{P}_g \]

\[ \vec{P}_g = (\varepsilon(\omega, k) - \varepsilon_0 \mathbf{I}) \langle \vec{E} \rangle \]

For a local medium:

\[ D = \varepsilon_0 \langle \mathbf{E} \rangle + \mathbf{P} \]
\[ \mathbf{H} = \frac{\langle \mathbf{B} \rangle}{\mu_0} - \mathbf{M} \]

\[ D = \varepsilon_0 \varepsilon_r \langle \mathbf{E} \rangle + \sqrt{\varepsilon_0 \mu_0} \xi \cdot \mathbf{H} \]
\[ \langle \mathbf{B} \rangle = \sqrt{\varepsilon_0 \mu_0} \zeta \cdot \langle \mathbf{E} \rangle + \mu_0 \mu_r \cdot \mathbf{H} \]

\[ \mathbf{P} = \varepsilon_0 (\varepsilon_r - \mathbf{I}) \cdot \langle \mathbf{E} \rangle + \frac{1}{\mu_0 c} \xi \cdot \mu_r^{-1}. \left( \langle \mathbf{B} \rangle - \frac{1}{c} \zeta \cdot \langle \mathbf{E} \rangle \right) \]

\[ \mathbf{M} = \frac{1}{\mu_0 c} \mu_r^{-1} \cdot \xi \cdot \langle \mathbf{E} \rangle + \frac{1}{\mu_0} \left( \mathbf{I} - \mu_r^{-1} \right) \cdot \langle \mathbf{B} \rangle \]
Relation between local and nonlocal parameters (contd.)

But since,

\[ P_g = P + \nabla \times \mathbf{M} / j\omega + \ldots \]

\[ \langle \mathbf{B} \rangle = \frac{k}{i\omega} \times \langle \mathbf{E} \rangle \]

it is found that:

\[
\frac{\varepsilon}{\varepsilon_0} (\omega, \mathbf{k}) = \left( \varepsilon_r - \xi \mu_r^{-1} \zeta \right) + \left( \xi \mu_r^{-1} \times \frac{c \mathbf{k}}{\omega} - \frac{c \mathbf{k}}{\omega} \times \mu_r^{-1} \zeta \right) + \frac{c \mathbf{k}}{\omega} \times \left( \mu_r^{-1} - \mathbf{I} \right) \times \frac{c \mathbf{k}}{\omega}
\]
Some remarks

• A local material can be characterized using the traditional constitutive relations as well as the “nonlocal” constitutive relations. For unbounded media, both phenomenological models predict the same physics.

• In particular, the plane wave solutions and macroscopic electric and induction fields are independent of the considered model.

• The nonlocal dielectric function can be obtained from the local parameters using the formula:

$$\frac{\varepsilon}{\varepsilon_0}(\omega, \mathbf{k}) = \left(\varepsilon_r - \xi \cdot \mu_r^{-1} \cdot \zeta\right) + \left(\xi \cdot \mu_r^{-1} \times \frac{c \mathbf{k}}{\omega} - \frac{c \mathbf{k}}{\omega} \times \mu_r^{-1} \cdot \zeta\right) + \frac{c \mathbf{k}}{\omega} \times \left(\mu_r^{-1} - \mathbf{I}\right) \times \frac{c \mathbf{k}}{\omega}$$
Some remarks (contd.)

- **It should also be clear that a material is local** (and such that, with the exception of the dipole moments, all the multipoles moments are negligible) **only if the nonlocal dielectric function is a quadratic form of the wave vector.**

\[
\frac{\varepsilon}{\varepsilon_0} (\omega, \mathbf{k}) = \left( \varepsilon_r - \xi \mu_r^{-1} \cdot \zeta \right) + \left( \xi \mu_r^{-1} \times \frac{c \mathbf{k}}{\omega} - \frac{c \mathbf{k}}{\omega} \times \mu_r^{-1} \cdot \zeta \right) + \frac{c \mathbf{k}}{\omega} \times \left( \mu_r^{-1} - \mathbf{I} \right) \times \frac{c \mathbf{k}}{\omega}
\]
How to extract the local parameters from the nonlocal dielectric function?

- The local parameters can be meaningful only if (weak spatial dispersion):

\[
\varepsilon(\omega, k) \approx \varepsilon(\omega, 0) + \sum_n \frac{\partial \varepsilon}{\partial k_n} (\omega, 0) k_n + \frac{1}{2} \sum_{n,m} \frac{\partial^2 \varepsilon}{\partial k_n \partial k_m} (\omega, 0) k_n k_m
\]
How to extract the local parameters from the nonlocal dielectric function? (contd.)

\[
\varepsilon(\omega, k) \approx \varepsilon(\omega, 0) + \sum_n \frac{\partial \varepsilon}{\partial k_n}(\omega, 0) k_n + \frac{1}{2} \sum_{n,m} \frac{\partial^2 \varepsilon}{\partial k_n \partial k_m}(\omega, 0) k_n k_m
\]

- The magnetoelectric tensors are related to the first order derivatives of the dielectric function.
- The magnetic permeability is related to the second order derivatives of the dielectric function.
Local permittivity:

Very simple:

\[
\varepsilon_r - \xi \cdot \mu_r^{-1} \cdot \zeta = \frac{\varepsilon}{\varepsilon_0} (\omega, 0)
\]

(but we also need to know the magnetoelastic tensors and permeability...)

Materials with a centre of inversion symmetry:

\[
\varepsilon_r(\omega) = \frac{\varepsilon}{\varepsilon_0} (\omega, 0)
\]
Magnetoelectric tensors:

\[ \varepsilon(\omega, k) \approx \varepsilon(\omega, 0) + \sum_n \frac{\partial \varepsilon}{\partial k_n}(\omega, 0) k_n + \frac{1}{2} \sum_{n,m} \frac{\partial^2 \varepsilon}{\partial k_n \partial k_m}(\omega, 0) k_n k_m \]

It can be verified that for dielectric inclusions, the first order derivatives are anti-symmetric tensors.

\[ \frac{\partial \varepsilon}{\partial k_x}, \frac{\partial \varepsilon}{\partial k_y}, \frac{\partial \varepsilon}{\partial k_z} \rightarrow 3 \times 3 = 9 \text{ independent parameters} \]
Magnetoelectric tensors (contd.):

\[ \xi = -\zeta^t \]

\[ \zeta = \mu_r \cdot \frac{\omega}{c} \sum_n \left( j q_n \hat{u}_n - \frac{1}{2} j q_n \cdot \hat{u}_n \mathbb{I} \right) \]

\[ j q_n = \frac{1}{2} \sum_m \frac{1}{\varepsilon_0} \hat{u}_m \cdot \frac{\partial \varepsilon}{\partial k_n} (\omega, 0) \times \hat{u}_m \]

Spatial dispersion of first order can be described exactly using the local model.
Magnetic Permeability:

\[
\frac{1}{2} \sum_{n,m} \frac{\partial^2 \varepsilon}{\partial k_n \partial k_m} (\omega, 0) k_n k_m \quad \equiv \quad \frac{c_k}{\omega} \times \left( \mu_r^{-1} - I \right) \times \frac{c_k}{\omega}
\]

How to choose \( \mu \) such that this is true?

It can be verified that for dielectric inclusions, the second order derivatives are symmetric tensors.

A problem:

\[
\frac{\partial^2 \varepsilon}{\partial k_x^2}, \frac{\partial^2 \varepsilon}{\partial k_y^2}, \frac{\partial^2 \varepsilon}{\partial k_z^2}, \frac{\partial^2 \varepsilon}{\partial k_x \partial k_y}, \frac{\partial^2 \varepsilon}{\partial k_x \partial k_z}, \frac{\partial^2 \varepsilon}{\partial k_y \partial k_z}
\]

\[6 \times 6 = 36\] independent parameters
Why such problem?

More rigorously,

\[ P_g = P + \nabla \times M / j\omega + \ldots \]

\[ P_g = P + \frac{1}{j\omega} \nabla \times M - \frac{1}{2} \nabla Q + \frac{1}{6} \nabla \nabla Q - \frac{1}{j\omega 2} \nabla \times \nabla S \]

\( Q, O \) - electric quadrupole and octopole moments

\( S \) - magnetic quadrupole moment

**Spatial dispersion of second order is not only due to the magnetic polarization, but also due to the quadrupole moments**
Solutions?

\[ \frac{1}{2} \sum_{n,m} \frac{\partial^2 \varepsilon}{\partial k_n \partial k_m} (\omega, 0) k_n k_m = \frac{c k}{\omega} \times \left( \mu_r^{-1} - I \right) \times \frac{c k}{\omega} \]

Too many scalar equations (36) and only a few scalar unknowns (6)...

Possibilities:

- **Consider only a small subset of the available equations...**
- Least square solution...
- Extract the effective parameters associated with quadrupole moments (too complicated!)
Example: Composite medium with SRRs and metallic wires

“Local” parameters:

\[
\mu_r(\omega) = \hat{u}_x \hat{u}_x + \hat{u}_y \hat{u}_y + \mu_{zz} \hat{u}_z \hat{u}_z
\]

\[
\varepsilon_r(\omega) = \varepsilon_{r,xx} \hat{u}_x \hat{u}_x + \varepsilon_{r,yy} \hat{u}_y \hat{u}_y + \hat{u}_z \hat{u}_z
\]
Extraction of the “local” parameters:

Assuming,

\[
\varepsilon_r(\omega) = \varepsilon_{r,xx} \hat{u}_x \hat{u}_x + \varepsilon_{r,yy} \hat{u}_y \hat{u}_y + \hat{u}_z \hat{u}_z
\]

\[
\mu_r(\omega) = \hat{u}_x \hat{u}_x + \hat{u}_y \hat{u}_y + \mu_{zz} \hat{u}_z \hat{u}_z
\]

We obtain,

\[
\varepsilon_r(\omega) = \lim_{k \to 0} \frac{\varepsilon}{\varepsilon_0}(\omega,\mathbf{k})
\]

\[
\mu_{zz}(\omega) = \frac{1}{1 - \beta^2 \frac{1}{2\varepsilon_0} \frac{\partial^2 \varepsilon_{yy}}{\partial k_x^2} \bigg|_{k=0}}
\]
Extracted parameters (I):

\[ \varepsilon_{yy} = 0.5 \]
\[ z = 0.01 \]
\[ w = 0.4 \]
\[ \text{med} = 0.125 \]

\( r_w = 0.01a \)
\( a_x = a_y = a \)
\( a_z = 0.5a \)
\( R_{\text{med}} = 0.4a \)
\( d = 0.125a \)
Band structure:

\[ \frac{\omega}{a} = 0.5 \]

\[ \omega = 0.01 \]

\[ w = 0.4 \]

\[ \text{med} Ra = 0.125 \]

\[ d = 0.125a \]

\[ r_w = 0.01a \]

\[ a_x = a_y \equiv a \]

\[ a_z = 0.5a \]

\[ R_{med} = 0.4a \]
Band structure:

\[ r_w = 0.01a \]
\[ a_x = a_y = a \]
\[ a_z = 0.5a \]
\[ R_{med} = 0.4a \]
\[ d = 0.125a \]

b)- only MSRR
Extracted parameters (II):

- Elliptical MSRR+Wires
- Only elliptical MSRR
- Only wires

\[
\begin{align*}
    x_{aa} & = x^2 \\
    y_{aa} & = 0.5 \\
    z_{aa} & = 0.4 \\
    x_R & = 0.125 \\
    d & = 0.01 \\
    w_R & = 0.8 \\
    R_y & = 0.8a \\
    r_w & = 0.01a \\
    d & = 0.125a
\end{align*}
\]
Band Structure:

a)- Elliptical MSRR+Wires

\[ a_x = a \]
\[ a_y = 2a \]
\[ a_z = 0.5a \]
\[ R_x = 0.4a \]
\[ R_y = 0.8a \]
\[ r_w = 0.01a \]
\[ d = 0.125a \]
b)- only elliptical MSRR

\[ a_x = a \]
\[ a_y = 2a \]
\[ a_z = 0.5a \]
\[ R_x = 0.4a \]
\[ R_y = 0.8a \]
\[ r_w = 0.01a \]
\[ d = 0.125a \]
Extracted parameters (III) (metasolenoid):

- $r_w = 0.01a$
- $a_x = a_y \equiv a$
- $a_z = 0.25a$
- $R_{med} = 0.4a$
- $d = 0.125a$
Band Structure:

\[
\begin{align*}
\omega &= 0.25a \\
a_x &= a_y = a \\
a_z &= 0.25a \\
R_{med} &= 0.4a \\
d &= 0.125a
\end{align*}
\]
Example II: Array of Helices

\[
\frac{\overline{\varepsilon_{\text{eff}}}}{\varepsilon_0} = \begin{pmatrix}
\varepsilon_t - \frac{A^2 k_x^2}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & \frac{A^2 k_x k_y}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & \frac{j A k_y}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} \\
\frac{A^2 k_x k_y}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & \varepsilon_t - \frac{A^2 k_y^2}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & \frac{-j A k_x}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} \\
\frac{j A k_y}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & \frac{-j A k_x}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} & 1 - \frac{1}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}}
\end{pmatrix}
\]
Local parameters (propagation in xoy plane)

\[
\overline{\mu_r} = \hat{u}_x \hat{u}_x + \hat{u}_y \hat{u}_y + \mu_{zz} \hat{u}_z \hat{u}_z \\
\mu_{zz} = \left(1 + \frac{\beta^2 A^2}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}}\right)^{-1} \\
\overline{\zeta} = \zeta_{zz} \hat{u}_z \hat{u}_z = -\frac{j \beta A}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} \\
\mu_{zz}^{-1} \zeta_{zz} = -\frac{j \beta A}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} \\
\overline{\epsilon_r} = \epsilon_t (\hat{u}_x \hat{u}_x + \hat{u}_y \hat{u}_y) + \epsilon_{zz} \hat{u}_z \hat{u}_z \\
\epsilon_{zz} = 1 - \frac{1}{\beta^2 / \beta^2_{p1} - k_z^2 / \beta^2_{p2}} - \frac{\zeta_{zz}^2}{\mu_{zz}}.
\]
Local parameters (propagation in xoy plane) (contd.)

Fig. 3. Effective parameters ($k_z = 0$) for a material with $R = 0.4a$, $r_w = 0.01a$, $p = 0.5a$. 

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May 5, Marrakech, 2008
Application of the local parameters in a scattering problem (using classical boundary conditions)

Fig. 8. Axis ratio of the transmitted wave as function of the normalized frequency. Solid lines: Analytical model; Diamond/Triangle/Star symbols: Full wave results. The radius of the helices is $R = 0.4a$. The wire radius, helix pitch, and the number of layers are: (a) $r_w = 0.01a$, $p = 0.5a$, $N_L = 5$, (b) $r_w = 0.01a$, $p = 0.9a$, $N_L = 5$, (c) $r_w = 0.05a$, $p = 0.9a$, $N_L = 3$. 
Problems involving interfaces
Problems involving interfaces of spatially dispersive media are difficult to solve…
Problems:

• The dielectric function is only defined for an unbounded periodic medium.

• The dielectric function is defined in spectral domain, but a problem involving interfaces is formulated in space domain.

\[ \varepsilon(\omega, \mathbf{k}) \rightarrow \text{Only makes sense in the spectral domain} \]

\[ \mathbf{E}(\mathbf{r}) \rightarrow \text{Only makes sense in the space domain} \]

k and r are dual Fourier variables and cannot appear in the same expression!
Problems (contd.):

**Maxwell’s equations in the space domain for a spatially dispersive material:**

\[ \nabla \times \langle E \rangle = -j\omega\mu_0 H_g \]

\[ \nabla \times H_g = \langle J_e \rangle + j\omega \int \hat{E}(r - r') \langle E \rangle(r') d^2r' \]

(valid only for unbounded periodic materials!; we do not even know how to extend this expression for finite blocks of a material!)

Quite scary!
Some reasonable assumptions:

For plane wave incidence, the field inside the nonlocal material is written in terms of the plane waves modes supported by the unbounded periodic material.
• In general, a spatially dispersive material may support “new waves”, as compared to the ordinary case in which only two plane waves are supported for a fixed direction of propagation.

• These extra degrees of freedom associated with spatially dispersive materials may prevent us from being able to solve a simple scattering problem, even if the dielectric function of the material is known!!!
An example: the wire medium

\[
\varepsilon_{zz}(\omega, k_z) = 1 - \frac{\beta_p^2}{(\omega/c)^2 - k_z^2}
\]

\[k = (k_x, k_y, k_z)\]
Electromagnetic modes in the wire medium:

- **TE-z modes**: electric field is normal to the wires; wires are transparent to the wave.

\[ k_{z,TE} = \sqrt{\left(\frac{\omega}{c}\right)^2 - k_x^2 - k_y^2} \]

- **TM-z modes**: magnetic field is normal to the wires; the mode is cut-off for long wavelengths.

\[ k_{z,TM} = -j \sqrt{\beta_p^2 + k_x^2 + k_y^2 - \left(\frac{\omega}{c}\right)} \]

- **TEM dispersionless modes** (transmission line modes).

\[ k_{z,TEM} = \left(\frac{\omega}{c}\right) \]
Is the permittivity model useful to solve a scattering problem?

Homogenized Wire Medium Slab

2 distinct polarizations

3 distinct polarizations

\[ \varepsilon_{zz}(\omega, k_z) = 1 - \frac{\beta_p^2}{(\omega/c)^2 - k_z^2} \]

The scattering problem cannot be solved
Additional Boundary Conditions
The ABC concept

• In order that to obtain the solution of a scattering problem using homogenization methods, it is necessary to specify boundary condition for the internal variables that describe the excitations responsible for the spatial dispersion effects.

• The nature of the ABC depends on the specific microstructure of the material, and can be determined only on the basis of a microscopic model that describes the dynamics of the internal variables.
The wire medium case:

The current along the wires must vanish at the interface.

It can be proved that this implies that the following additional boundary condition is verified:

\[
\varepsilon_0 E_z \bigg|_{\text{air side}} = \varepsilon_{host} E_z \bigg|_{\text{wire medium side}}
\]
Some considerations about the ABC:

Is the ABC compatible/equivalent with the continuity of the normal component of the electric displacement $D$?

\[
E(r) = \sum_i c_i E_{av,i}(r;k_i)
\]

\[
D(r) = \sum_i c_i \varepsilon(\omega, k_i) E_{av,i}(r;k_i)
\]

Thus, $\varepsilon_{host} E$ is not collinear with $D$

There is no contradiction/redundancy between the new ABC and the continuity of the normal component of $D$.
\[ H_x = (e^{-\gamma_0 z} + \rho e^{+\gamma_0 z})e^{-jk_y y} \quad \text{(air side: } z < 0) \]

\[ H_x = (B_1^+ e^{-j\beta_h z} + B_1^- e^{+j\beta_h z} + B_2^+ e^{-\gamma_{TM} z} + B_2^- e^{+\gamma_{TM} z})e^{-jk_y y} \]

\quad \text{(wire medium: } 0 < z < L) \]

\[ H_x = t e^{-\gamma_0 (z-L)}e^{-jk_y y} \quad \text{(air side: } z > L) \]

**Boundary conditions:**

\[
\begin{align*}
[H_x] &= 0; \quad \left[\varepsilon^{-1}_{h} dH_x/dz\right] = 0 \\
[\frac{d^2 H_x}{dz^2}] &= - (\beta_h^2 - \beta^2) H_x.
\end{align*}
\]
Example (contd.):

\[ r_w = 0.01a \]

\[ \theta_i = 45[\text{deg}] \]
Application to the characterization of wire medium lenses

30 THz

$$\varepsilon_{Ag} = -5143 - j746$$

$$a = 215\,nm \quad (\beta a = 0.2)$$

$$\varepsilon_h = 2.2 \ (\text{Halcogenide glass})$$

$$R = 21.5\,nm$$

$$L = 5.93\,\mu m$$
Imaging at infrared frequencies:
Imaging at 30THz:

Front interface

Back interface

a) 

b)
ABC for a WM connected to a ground plane:

The microscopic density of charge must vanish at the connection point.
ABC for a WM connected to a ground plane (contd.):

\[
\left( k_{||} \hat{u}_\alpha + \hat{u}_z \hat{u}_\alpha j \frac{d}{dz} \right) \left( \omega \varepsilon_0 \varepsilon_h \hat{u}_\alpha \cdot E + \hat{u}_\alpha \times \left( k_{||} + \hat{u}_z j \frac{d}{dz} \right) \cdot H \right) = 0
\]
FIGURE 1.11  Reflection characteristic for a substrate formed by tilted wires ($\alpha = 45[\text{deg}]$) connected to a PEC plane. The wires are embedded in a dielectric with $\varepsilon_r = 4.0$ and thickness $T$ such that $T \sqrt{\varepsilon_r \omega / c} = \pi / 4$. The spacing between the wires, $a$, associated with each curve is indicated in the figure. The radius of the wires is $r_w = 0.05a$, and the length of the wires is $L_w = T \sec \alpha$. The solid lines were
Application: HIS (contd.)

\[ \text{eps}_h = 1 \]
\[ g = 0.1a \quad \text{(distance between patches)} \]
\[ h = 5a \]
\[ r = 0.05a \]
\[ \text{Angle of incidence: 45 degree} \]

Phase of \( \rho \) as function of \( \omega a/c \)
It is also possible to derive ABCs for other more complex WM:

The number of required ABCs may be 1, 2 or 3!!!