Advanced Electromagnetics:  
21st Century Electromagnetics

Homogenization & Parameter Retrieval

Lecture Outline

• Introduction
• Nicolson-Ross-Weir method
• Alternate S-parameter retrieval method
• Homogenization by field averaging
• T-matrix parameter retrieval
• Parameter retrieval through optimization
• Low frequency methods
• Refractive index retrieval through phase response
• Homogenization of photonic crystals
• Conclusion
• Appendix
  • S parameters from a vector network analyzer
What is Parameter Retrieval and Homogenization?

A metamaterial slab produces some complex reflection and transmission response.

A homogeneous slab of the same thickness produces the same complex reflection and transmission response.

These are the effective, or homogenized, material properties of the metamaterial.
Usefulness of Homogenization

#1
Knowing the effective properties allows you realize crazy designs, like those designed from spatial transforms.

#2
Preliminary simulations using just the effective properties are more efficient because they do not require fine meshing.

The Problem ➔ Branching

we have multiple correct solutions for each choice of $d$. 

\[
\text{Error} = \sqrt{(R_{\text{meta}} - R_{\text{homo}})^2 + (T_{\text{meta}} - T_{\text{homo}})^2}
\]
Degrees of Freedom

A material is commonly characterized by either the complex permittivity and permeability or by the complex refractive index and impedance.

\[
\begin{align*}
\mu_r &= \mu' + j \mu'' \\
\epsilon_r &= \epsilon' + j \epsilon'' \\
\eta_r &= \eta' + j \eta'' \\
n &= n' + j n''
\end{align*}
\]

We see that four real numbers are needed to completely describe a material.

For this reason, four measurements are needed in order to completely calculate the material properties.

\[
\begin{align*}
S_{11} &= \text{Re}[S_{11}] + j \text{Im}[S_{11}] \\
S_{21} &= \text{Re}[S_{21}] + j \text{Im}[S_{21}]
\end{align*}
\]

Other possible combinations include measurements at different polarizations, different angles, etc.

Notes on Homogenization

• Complicated due to branching
• No “best” method
• Does not work well for longitudinally resonant devices
• Homogenization does not always apply to photonic crystals that diffract and scatter waves.
Nicholson-Ross-Weir Method

References:

Basic Concept of S-Parameter Retrieval

It is possible to conceptually replace an inhomogeneous structure with a continuous structure without changing the scattering characteristics (magnitude and phase of both reflection and transmission).

\[ S_{III} = S_{II} \]
Flow of Parameter Retrieval

The scattering parameters are either measured or modeled.

From the scattering parameters, the complex refractive index and impedance is calculated. This is a complicated step.

Finally, the complex permittivity and permeability is calculated.

Scattering Analysis (1 of 2)

Here we distinguish between scattering at a single interface and scattering from the unit cell.
Scattering Analysis (2 of 2)

Overall reflection is the sum of all reflected waves. Overall transmission is the sum of all transmitted waves. These summations are geometric series and can be written in closed form with summations.

For parameter retrieval, we start formulating our algorithm by inverting these equations to solve for \( r \) and \( t \).

\[
S_{11} = \frac{(1 - t^2)r}{1 - r^2t^2}
\]
\[
S_{21} = \frac{(1 - r^2)t}{1 - r^2t^2}
\]
\[
r = \frac{\eta - \eta_0}{\eta + \eta_0}
\]
\[
t = e^{j\kappa_0nd}
\]

\[
X = \frac{1 - S_{21}^2 + S_{11}^2}{2S_{11}}
\]
\[
r = X \pm \sqrt{X^2 - 1}
\]
\[
t = \frac{S_{11} + S_{21} - r}{1 - (S_{11} + S_{21})r}
\]

\( r, t \rightarrow S_{11, S_{21}} \)

\( S_{11, S_{21}} \rightarrow r, t \)
Resolve Sign Ambiguity

For passive materials, the reflection coefficient must be less than or equal to one.

\[ r = X \pm \sqrt{X^2 - 1} \]

Choose \( \pm \) such that \( |r| \leq 1 \)

Why?: If \( |r| > 0 \), this implies that more power is reflecting from the interface than is incident upon it. This is impossible for passive materials (i.e. no gain) due to conservation of power.

Solve for Material Properties (Nicolson-Ross Method)

Now that the reflection coefficient \( r \) is known, we can extract impedance \( \eta \) from it.

\[ r = \frac{\eta - \eta_0}{\eta + \eta_0} \quad \rightarrow \quad \eta = \eta_0 \frac{1 + r}{1 - r} \]

Moreover, refractive index \( n \) can be extracted from the parameter \( t \).

\[ t = e^{jk_0nd} \quad \rightarrow \quad n = \frac{\ln t}{jk_0d} \]
Branching Problem

Strictly speaking, the following inversion is not correct

\[ t = e^{jk_0nd} \rightarrow n = \frac{\ln t}{jk_0d} \]

because \( \ln(e^{jk_0nd}) \neq jk_0nd \).

\[ \ln(e^{jk_0nd}) = j(k_0nd + 2\pi m) \]

Sines and cosines give the same angle when any integer multiple of \( 2\pi \) is added or subtracted to the angle argument. This is called “branching” and it means there are an infinite number of correct answers.

The NRW method assumes a thin (usually \( \lambda/4 \)) sample such that \( m = 0 \).

---

Extract \( \mu_r \) and \( \varepsilon_r \)
(Nicolson-Ross Method)

We first invert our basic equations relating \( n \) and \( \eta \) to \( \mu_r \) and \( \varepsilon_r \).

\[ \eta = \eta_0 \sqrt{\frac{\mu_r}{\varepsilon_r}} \rightarrow \mu_r = \left( \frac{\eta}{\eta_0} \right)^2 \]

\[ n = \sqrt{\mu_r \varepsilon_r} \rightarrow \mu_r \varepsilon_r = n^2 \]

Next, we separate \( \mu_r \) and \( \varepsilon_r \).

\[ \mu_r = n \frac{\eta}{\eta_0} \quad \varepsilon_r = n \frac{\eta_0}{\eta} \]
Setup for Waveguide Measurements

Weir modified the Nicolson-Ross method to extract material properties from measurements of samples inside waveguides.

Weir Modification for Waveguide Measurements

A waveguide is not a transmission line and it has a cutoff wavelength $\lambda_c$. The wavelength of the guided mode is

$$\frac{1}{\Lambda} = \sqrt{\frac{\mu_r \varepsilon_r}{\lambda_0^2} - \frac{1}{\lambda_c^2}} = \sqrt{-\left[ \frac{\ln (1/t)}{2\pi d} \right]^2} = \frac{\ln t}{j2\pi d}$$

Our equations for $\mu_r$ and $\varepsilon_r$ become

$$\mu_r = \frac{1}{\Lambda} \left(\frac{1+r}{1-r}\right) \sqrt{\frac{1}{\lambda_0^2} - \frac{1}{\lambda_c^2}}$$

$$\varepsilon_r = \frac{\lambda_0^2}{\mu_r} \left(\frac{1}{\Lambda^2} + \frac{1}{\lambda_c^2}\right)$$
Problem with Logarithm

The exponential has not been inverted correctly to account for branching.

\[ \ln \frac{1}{t} = \ln \left| \frac{1}{t} \right| + j \left( \frac{1}{t} + 2\pi m \right) \]

Weir interpreted \( m \) as the number of wavelengths within the sample thickness \( d \).

\[
 m \approx \text{floor} \left( \frac{d}{\lambda} \right) \\
 \lambda = \frac{\lambda_0}{\sqrt{1 - (\lambda_0 / \lambda_c)^2}}
\]

For a quarter-wave sample, \( d/\lambda = 0.25 \) so \( m = 0 \).
The final equations become what was on the previous slide.

Alternate S-Parameter Retrieval

References:
Parameter Retrieval

The scattering analysis calculated the scattering parameters from the material parameters $n$ and $\eta$.

\[
S_{11} = \frac{(1 - r^2)}{1 - r^2 t^2} \\
S_{21} = \frac{(1 - r^2 t)}{1 - r^2 t^2} \\
r = \frac{\eta - \eta_0}{\eta + \eta_0} \\
t = e^{jk_0nd}
\]

We can now calculate the material parameters from the scattering parameters by inverting the above equations.

\[
\eta = \pm \sqrt{(1 + S_{11})^2 - S_{21}^2} \\
\sqrt{(1 - S_{11})^2 - S_{21}^2} \\
t = X \pm \sqrt{1 - X^2} \\
X = \frac{1}{2S_{21}(1 - S_{11}^2 + S_{21}^2)}
\]

Assume Passive Materials

We will assume that we are working with a passive material. That is, the sample has no gain.

This implies that

- $\text{Re}[\eta] \geq 0$
- $\text{Im}[n] \geq 0$
- $\text{Im}[\mu_r] \geq 0$
- $\text{Im}[\varepsilon_r] \geq 0$

\[
\eta = R + jX \\
n = n_0 + jk \\
\mu_r = \mu'_r + j\mu''_r \\
\varepsilon_r = \varepsilon'_r + j\varepsilon''_r
\]

- Resistive part of impedance must be positive to not imply gain.
- Extinction coefficient must be positive for decay.
- Imaginary component must be positive to convey loss and not gain.
- Imaginary component must be positive to convey loss and not gain.
Sign of Impedance

How do we resolve the sign of the impedance?

\[ \eta = \pm \sqrt{\frac{(1 + S_{11})^2 - S_{21}^2}{(1 - S_{11})^2 - S_{21}^2}} \]

We choose the sign that makes the impedance consistent with passive materials.

\[ \text{Re}[\eta] \geq 0 \]

Calculating the Transmission Coefficient $t$

Given the impedance with resolved sign, we can calculate the transmission coefficient without sign ambiguity using the following equation.

\[ t = \frac{S_{21}}{1 - S_{11}r} \]
Retrieving the Refractive Index

We retrieve the refractive index from $t$, but we must invert the exponential.

First, we write the refractive index as a complex number.

$$t = e^{jk_0(n' + jn')d} = e^{jk_0n'd} e^{-k_0n'd}$$

Second, we calculate the natural log of this equation.

$$\ln t = \ln(e^{jk_0n'd} e^{-k_0n'd}) = \ln(e^{jk_0n'd}) + \ln(e^{-k_0n'd})$$

$$= \ln(e^{jk_0n'd}) - k_0n'd$$

How do we calculate this term?

Branching

What is $\cos^{-1}(0.5)$? There is actually an infinite number of correct answers!

$$\cos^{-1}(0.5) = 60^\circ + (360^\circ)m \quad m = -\infty, \ldots, -2, -1, 0, 1, 2, \ldots, \infty$$

We must apply this concept to invert the complex exponential.

$$\ln(e^{jk_0n'd}) = j(k_0n'd - 2\pi m)$$

Since $m$ is any integer, we are free to write whatever sign is convenient here.
Retrieved Complex Refractive Index

We must apply this concept to invert the complex exponential.

\[ \ln t = \ln(e^{jk_0n''d}) - k_0n''d \]
\[ = j(k_0n'd - 2\pi m) - k_0n''d \]

From this expression, we assemble the complex refractive index.

\[ \text{Re}[\ln t] = -k_0n''d \quad n' = \frac{1}{k_0d}(\text{Im}[\ln t] + 2\pi m) \]
\[ \text{Im}[\ln t] = k_0n'd - 2\pi m \quad n'' = \frac{1}{k_0d}\text{Re}[\ln t] \]

We can now calculate \( n'' \) without problems, but we must resolve the branching problem to determine the correct \( n' \).

Resolving the Branching (1 of 2)

Given the refractive index at the first frequency \( n(f_0) \), we can express the refractive index at the second frequency \( n(f_1) \) using a Taylor series. This is done to ensure the refractive index function is smooth and continuous.

\[ e^{j\frac{k_0}{\lambda}n(f_1)d} = e^{j\frac{k_0}{\lambda}n(f_0)d} \left[ 1 + \Delta + \frac{\Delta^2}{2} + \cdots \right] \]
\[ \Delta = jk_0(f_1)n(f_1)d - jk_0(f_0)n(f_0)d \]

The only unknown in this equation is the branch index \( m \) that occurs in the real part of \( n(f_1) \) on the left hand side.
Resolving the Branching (2 of 2)

The equation on the previous slide is a binomial function of the unknown \( n(f_1) \) and has two possible solutions.

\[
e^{j\phi_0(f_1)n(f_1)d} = e^{j\phi_0(f_1)n(f_1)d} \left[ 1 + \Delta + \frac{\Delta^2}{2} + \cdots \right] \rightarrow n(f_1)_{\text{Root } #1} \text{ or } n(f_1)_{\text{Root } #2}
\]

We can calculate the imaginary part \( n(f_1) \) without ambiguity. We choose the above root with an imaginary part that most closely matches.

We now have a good approximation of the refractive index. To calculate exactly, we choose \( m \) that yields the closest refractive index to the above approximation.

\[
n' = \frac{1}{k_0d} \left( \text{Im}[\ln t] + 2\pi m \right) \quad n'' = -\frac{1}{k_0d} \text{Re}[\ln t]
\]

Resolving the Branching at the First Frequency Point (1 of 2)

The constitutive parameters \( \mu_r \) and \( \varepsilon_r \) are calculated from \( n \) and \( \eta \) as follows.

\[
\mu_r = n\eta \quad \varepsilon_r = \frac{n}{\eta}
\]

The imaginary parts of \( \mu_r \) and \( \varepsilon_r \) are then

\[
\mu'' = n'\eta'' + n''\eta' \quad \varepsilon'' = \frac{1}{|\eta|} (-n'\eta'' + n''\eta')
\]

If the material is passive, then \( \mu'' \geq 0, \varepsilon'' \geq 0 \) which implies

\[
|n'\eta''| \leq n''\eta'
\]
Resolving the Branching at the First Frequency Point (2 of 2)

We choose the branch index $m$ that satisfies the condition for a passive materials.

$$|n'\eta''| \leq n''\eta'$$

We now have two possible situations.

1. Only one solution for $m$ exists. That is the correct answer.
2. Multiple solutions exist. For each branch $m$, we calculate the refractive index for all other frequencies. The correct choice for the initial branch $m$ will produce a refractive index function that satisfies the above relation for all frequencies.

Example: Negative Index Medium

FIG. 8. Retrieved $\epsilon$, $\mu$, and $\mu'$ (real and imaginary parts) for a one-cell metamaterial structure taken from Refs. [14,21] and shown in the inset (a). The vertical dashed lines denote the limits of the resonance band.
Homogenization by Field Averaging

References:

Benefits and Drawbacks

• Benefits
  • Resolves the branching problem quite easily
  • Accurate

• Drawbacks
  • Computationally more intensive
  • Essentially requires a simulation
Homogenization by Field Averaging

First, given a Bloch wave vector, the Bloch mode is calculated. This gives the field throughout the unit cell.

Second, the fields are averaged at points on the surface that correspond to points on the Yee grid.

Third, the average effective material parameters are extracted from the constitutive relations using the averaged field quantities.

Fourth, the effective material properties are calculated from the average effective material properties by removing grid dispersion.

Stoke’s Theorem

Stoke’s theorem comes from vector calculus and can be used to convert a surface integral into a line integral enclosing the surface.

\[
\oint_L \vec{A} \cdot d\vec{l} = \iint_S (\nabla \times \vec{A}) \cdot d\vec{s}
\]
Integrate Maxwell’s Equations

Start with the following of Maxwell’s equations.

\[
\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = j\omega B_x
\]

This could be integrated over the \( x = 0 \) surface.

\[
\iint_{x=0} \left( \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right) dydz = \iint_{x=0} j\omega B_x dydz
\]

Instead, the surface integral on the left side of this equation is converted to a line integral using Stoke’s theorem.

\[
\int_{0}^{a} E_z(0,0,z) dz + \int_{0}^{a} E_y(0,y,a) dy - \int_{0}^{a} E_z(0,a,z) dz - \int_{0}^{a} E_y(0,y,0) dy = j\omega \int_{0}^{a} B_y(0,y,z) dydz
\]
Interpret Terms as Field Averages

Now “average” field quantities can be defined.

\[
\int_0^z E_z(0,0,z)\,dz - \int_0^z E_z(0,a,z)\,dz - \int_0^y E_y(0,y,0)\,dy + \int_0^y E_y(0,y,a)\,dy = j\omega \int_0^y B_y(0,y,z)\,dy\,dz
\]

\[
\bar{E}_z\left(0,\frac{a}{2}\right) = \frac{1}{a} \int_0^z E_z(0,0,z)\,dz
\]

\[
\bar{E}_z\left(0,a,\frac{a}{2}\right) = \frac{1}{a} \int_0^z E_z(0,a,z)\,dz
\]

\[
\bar{E}_z\left(0,\frac{a}{2},0\right) = \frac{1}{a} \int_0^y E_y(0,y,0)\,dy
\]

\[
\bar{E}_z\left(0,\frac{a}{2},a\right) = \frac{1}{a} \int_0^y E_y(0,y,a)\,dy
\]

We average the \( E \) fields using line integrals.

We average the \( B \) fields using surface integrals.

Write Maxwell’s Equation in Terms of Averaged Fields

The equation can now be written using the averaged field quantities.

\[
\int_0^z E_z(0,0,z)\,dz - \int_0^z E_z(0,a,z)\,dz - \int_0^y E_y(0,y,0)\,dy + \int_0^y E_y(0,y,a)\,dy = j\omega \int_0^y B_y(0,y,z)\,dy\,dz
\]

\[
\downarrow
\]

\[
a\bar{E}_z\left(0,\frac{a}{2}\right) - a\bar{E}_z\left(0,a,\frac{a}{2}\right) - a\bar{E}_z\left(0,\frac{a}{2},0\right) + a\bar{E}_z\left(0,\frac{a}{2},a\right) = j\omega a^2 \bar{B}_z\left(0,\frac{a}{2},\frac{a}{2}\right)
\]

\[
\downarrow
\]

\[
\frac{\bar{E}_z\left(0,0,\frac{a}{2}\right) - \bar{E}_z\left(0,a,\frac{a}{2}\right)}{a} - \frac{\bar{E}_z\left(0,\frac{a}{2},0\right) - \bar{E}_z\left(0,\frac{a}{2},a\right)}{a} = j\omega \bar{B}_z\left(0,\frac{a}{2},\frac{a}{2}\right)
\]

This last equation is exactly the same as a finite-difference equation on a Yee grid!! Now lattice constant can be interpreted as the grid resolution.

\[a = \Delta x = \Delta y = \Delta z\]
Compute All Average Fields

This same procedure is applied to all six of Maxwell’s equations to derive equations for the average field quantities.

The average field quantities are defined to exist at the exact same points as they would on a Yee grid.

\[ \begin{align*}
\bar{E}_x, \bar{E}_y, \text{ and } \bar{E}_z \\
\bar{H}_x, \bar{H}_y, \text{ and } \bar{H}_z
\end{align*} \]

\[ \begin{align*}
\text{Calculated using line integrals along the edge where the field components exist.}
\end{align*} \]

\[ \begin{align*}
\bar{D}_x, \bar{D}_y, \text{ and } \bar{D}_z \\
\bar{B}_x, \bar{B}_y, \text{ and } \bar{B}_z
\end{align*} \]

\[ \begin{align*}
\text{Calculated using surface integrals across the surfaces where the field components exist.}
\end{align*} \]

Constitutive Relations

For “bi” media, the constitutive relations are

\[ \begin{align*}
\bar{D} &= \varepsilon_0 \left[ [\bar{\varepsilon}_r] \bar{E} - \frac{j}{c_0} [\kappa] \bar{H} \right] \\
\bar{B} &= \frac{j}{c_0} [\kappa]^T \bar{E} + \mu_0 [\bar{\mu}_t] \bar{H}
\end{align*} \]

Since all of the field quantities are now known, we solve for the average material properties from the constitutive relations.

\[ [\bar{\varepsilon}_r] \equiv \text{Averaged relative permittivity tensor} \]

\[ [\bar{\mu}_t] \equiv \text{Averaged relative permeability tensor} \]

\[ [\kappa] \equiv \text{Averaged magnetoelastic tensor} \]
Dispersion on a Yee Grid

Recall the dispersion relation for an isotropic material with parameters $\mu_r$ and $\varepsilon_r$.

$$\left(\frac{\omega}{c_0}\right)^2 \mu_r \varepsilon_r = \beta_x^2 + \beta_y^2 + \beta_z^2$$

The analogous dispersion relation on a frequency-domain Yee grid filled with $\mu_r$ and $\varepsilon_r$ is

$$\left(\frac{\omega}{v}\right)^2 \mu \varepsilon_r = \left[ \frac{2}{\Delta_x} \sin \left( \frac{\beta_x \Delta_x}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_y} \sin \left( \frac{\beta_y \Delta_y}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_z} \sin \left( \frac{\beta_z \Delta_z}{2} \right) \right]^2$$

In this equation, the speed of light $c_0$ is written as $v$ because the velocity changes due to the dispersion of the grid.

Recall that $a = \Delta x = \Delta y = \Delta z$.

Compensation Factor $\gamma$

The dispersion equation is solved for velocity $v$.

$$v = \omega \sqrt{\mu \varepsilon_r} \sqrt{\left[ \frac{2}{\Delta_x} \sin \left( \frac{\beta_x \Delta_x}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_y} \sin \left( \frac{\beta_y \Delta_y}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_z} \sin \left( \frac{\beta_z \Delta_z}{2} \right) \right]^2}$$

In the absence of grid dispersion, $v$ should be the speed of light $c_0$. Due to the Yee grid, it is slightly slower by a factor $\gamma$.

$$v = \gamma c_0$$

We can calculate this factor by combining the above equations.

$$\gamma = k_0 \sqrt{\mu \varepsilon_r} \sqrt{\left[ \frac{2}{\Delta_x} \sin \left( \frac{\beta_x \Delta_x}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_y} \sin \left( \frac{\beta_y \Delta_y}{2} \right) \right]^2 + \left[ \frac{2}{\Delta_z} \sin \left( \frac{\beta_z \Delta_z}{2} \right) \right]^2}$$
Remove Grid Dispersion

From the constitutive relations, the average effective material properties are calculated.

\[
\begin{bmatrix}
\bar{\mu}_r \\
\bar{\varepsilon}_r \\
\bar{k}
\end{bmatrix}, \quad \begin{bmatrix}
\varepsilon_{r,\text{eff}} \\
\mu_{r,\text{eff}} \\
\kappa_{\text{eff}}
\end{bmatrix}
\]

These terms incorporate grid dispersion from the Yee grid that must be removed to recover the effective material properties of the medium.

For dielectric materials, the average effective dielectric constant will be slightly larger than the true effective dielectric constant due to grid dispersion.

We remove the grid dispersion as follows:

\[
\varepsilon_{r,\text{eff}} = \gamma \bar{\varepsilon}_r
\]

Example 1: Maxwell-Garnett Medium

Fig. 2. Cubic lattice of dielectric spheres. (right) Close-up of a single unit cell of the array. The dielectric constant of the spheres is \( \varepsilon = 4 \).

Fig. 3. Effective permittivity and permeability of a cubic array of dielectric spheres, as a function of sphere radius. The dielectric constant of the spheres is \( \varepsilon = 4 \). The permeability values all start from zero frequency at unity and disperse downward with decreasing frequency. The permittivity values start from zero frequency in accordance with the Maxwell-Garnett formula and disperse upward with increasing frequency.
Example 2: Wire Medium

\[ \varepsilon_r(\omega) = 1 - \left( \frac{\omega_p}{\omega} \right)^2 \]  Eq. (31)

![Diagram of a wire medium](image)

Fig. 5. Retrieved values of permittivity (black curve) and permeability (gray curve) for the wire lattice. Because there are no propagating modes below the plasma frequency, the curves begin at the plasma frequency. The dots correspond to an S-parameter retrieval performed on an S-parameter calculation of the unit cell. The dashed curve corresponds to the ideal form for a plasmonic medium, Eq. (31).

Example 3: Split Ring Resonator Medium

![Diagram of SRRs](image)

Fig. 6. (a) Diagram of the SRRs and axes used in the simulation, \( a = 0.6 \mu m, t = 0.6 \mu m, \) and the line widths are 0.06 \( \mu m \), where \( a \) is the unit-cell length. (b) SRRs arranged asymmetrically. A structure composed of SRRs exhibits electric, magnetic, and magnetoelectric resonant responses. (c) SRRs arranged symmetrically. The restoration of mirror plane symmetry along the \( z \) axis eliminates the magnetoelectric coupling. (d) This arrangement of SRRs reduces the resonant electric and magnetoelectric responses.

Fig. 8. Retrieved permittivity and permeability for the SRR medium, oriented for primarily magnetic response.
T-Matrix Parameter Retrieval

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Transfer Matrix Algorithm

A transfer matrix relates fields on either side of a slab.

\[
\begin{bmatrix}
E_z(z) \\
E_z(z + d) \\
H_y(z) \\
H_y(z + d)
\end{bmatrix}
= T

\begin{bmatrix}
E_z(0) \\
E_z(0) \\
H_y(0) \\
H_y(0)
\end{bmatrix}
\]

\[\Rightarrow \psi_{\text{right}} = T \psi_{\text{left}}\]

If the T-matrix is for a unit cell of a longitudinally periodic structure, the following boundary condition must hold.

\[\psi_{\text{right}} = e^{jd} \psi_{\text{left}}\]

Substituting this into the T-matrix equation leads to an eigen-value problem from which the modes and propagation constants can be determined.

\[T \psi_{\text{left}} = e^{jd} \psi_{\text{left}}\]

\[\lambda = e^{jd}\]

\[\beta = k_n = \frac{\ln \lambda + 2\pi m}{jd}\]

There is still a branching problem here.
S-Matrix Algorithm (1 of 3)

An overall scattering matrix is calculated that describes the unit cell.

\[
\begin{bmatrix}
    c_{N+1}^- \\
    c_{N+1}^+
\end{bmatrix} =
\begin{bmatrix}
    S_{11}^{(\text{cell})} & S_{12}^{(\text{cell})} \\
    S_{21}^{(\text{cell})} & S_{22}^{(\text{cell})}
\end{bmatrix}
\begin{bmatrix}
    c_{0}^- \\
    c_{0}^+
\end{bmatrix}
\]

The terms are rearranged in “almost” the form of a transfer matrix.

\[
\begin{bmatrix}
    0 & -S_{12}^{(\text{cell})} \\
    I & -S_{22}^{(\text{cell})}
\end{bmatrix}
\begin{bmatrix}
    c_{N+1}^+ \\
    c_{N+1}^-
\end{bmatrix} =
\begin{bmatrix}
    S_{11}^{(\text{cell})} & -I \\
    S_{21}^{(\text{cell})} & 0
\end{bmatrix}
\begin{bmatrix}
    c_{0}^+ \\
    c_{0}^-
\end{bmatrix}
\]

If the device is infinitely periodic in the \(z\) direction, then the following periodic boundary condition must hold.

\[
\begin{bmatrix}
    c_{N+1}^+ \\
    c_{N+1}^-
\end{bmatrix} = e^{i\hat{k}_z A_z} \begin{bmatrix}
    c_{0}^+ \\
    c_{0}^-
\end{bmatrix}
\]

Here \(\hat{k}_z\) is the “effective” propagation constant of the mode.

S-Matrix Algorithm (2 of 3)

We substitute the periodic boundary condition into our rearranged equation to get

\[
\begin{bmatrix}
    S_{11}^{(\text{cell})} & -I \\
    S_{21}^{(\text{cell})} & 0
\end{bmatrix}
\begin{bmatrix}
    c_{0}^+ \\
    c_{0}^-
\end{bmatrix} = e^{i\hat{k}_z A_z} \begin{bmatrix}
    0 & -S_{12}^{(\text{cell})} \\
    I & -S_{22}^{(\text{cell})}
\end{bmatrix}
\begin{bmatrix}
    c_{0}^+ \\
    c_{0}^-
\end{bmatrix}
\]

This is a generalized eigen-value problem.

\[
Ax = \lambda Bx
\]

\[
A = \begin{bmatrix}
    S_{11}^{(\text{cell})} & -I \\
    S_{21}^{(\text{cell})} & 0
\end{bmatrix}, \\
B = \begin{bmatrix}
    0 & -S_{12}^{(\text{cell})} \\
    I & -S_{22}^{(\text{cell})}
\end{bmatrix}, \\
[V,D] = \text{eig}(A,B);
\]

\[
\lambda = e^{i\hat{k}_z A_z}
\]
S-Matrix Algorithm (3 of 3)

The eigen-value can also be written as
\[ \lambda = e^{ik_z \Lambda_z} = e^{i(k_0 n_{\text{eff}} \Lambda_z + 2\pi m)} \quad m \equiv \text{branching parameter} \]

Solving this for \( n_{\text{eff}} \) gives
\[ n_{\text{eff}} = \ln \frac{\lambda - 2\pi m}{k_0 \Lambda_z} \]

You will need to identify the eigen-value \( \lambda \) of the zero-order mode and calculate \( n_{\text{eff}} \) from it. Further, you will need to choose the branch parameter \( m \).

For thin slabs, \( m = 0 \) is usually the correct choice and avoids having to solve the branching problem.

z-Uniform Media

For media that are uniform in the \( z \) direction, the effective material parameters can be extracted from the eigen-values calculated from the zero-order mode in the cross section.

These are the eigen-values obtained in RCWA, MoL, waveguide analysis, and more.

For example, from RCWA...

\[ \frac{d^2}{dz^2} \begin{bmatrix} s_x \\ s_y \end{bmatrix} - \Omega^2 \begin{bmatrix} s_x \\ s_y \end{bmatrix} = 0 \]
\[ \Omega^2 = PQ \]
\[ W = \text{Eigen-vector matrix of } \Omega^2 \]
\[ \lambda^2 = \text{Eigen-value matrix of } \Omega^2 \]
\[ \begin{bmatrix} s_x(z) \\ s_y(z) \end{bmatrix} = W e^{-i\lambda z} + W e^{i\lambda z} \]

\[ n_{\text{eff}} = \sqrt{\Omega^2} \]
\[ \varepsilon_{\text{r,eff}} = n_{\text{eff}}^2 \]

Choose the eigen-value of the zero-order mode.
Parameter Retrieval Through Optimization

S-Parameter Optimization Approach

Optimization algorithms can also be used to determine effective material properties.

This approach is slower, but more versatile and can be used when no closed form equations exist.

This algorithm to the right is then iterated over frequency.

1. Make an initial guess at $\mu_r$ and $\varepsilon_r$.
3. Compare model to target scattering parameters. $\text{err} = |S_{\text{target}} - [S]|$.
4. Refine $\mu_r$ and $\varepsilon_r$.
5. Check if $\text{err} < \text{threshold}$.
   - Yes: Finished!
   - No: Go back to step 3.

Done when $\text{err} < \text{threshold}$.
Lorentz-Drude Model Optimization Approach

A Lorentz-Drude model approach sweeps frequency and then optimizes Lorentz-Drude parameters until a best fit is found.

Optical ellipsometry typically works this way.

We may sweep frequency, angle of incidence, polarization, etc.

Radio Frequency “Ellipsometry”

An NRL Arch for millimeter wave measurements

Calculating Effective Material Properties using PWEM

The effective refractive index of a periodic structure for a Bloch wave is easily calculated from the Bloch wave vector $\vec{\beta}$ and its frequency $k_0$.

$$|\vec{\beta}| = \frac{2\pi}{\lambda}$$

$$n_{\text{eff}} = \frac{|\vec{\beta}|}{k_0}$$

Note: Be sure to make $\vec{\beta}$ small for low-frequency parameter retrieval!
Polarization is Needed to Determine Tensor Components

When 3D PWEM is used, the two lowest-order bands will be calculated from which two effective refractive indices can be calculated.

These correspond to two modes with different polarizations.

In anisotropic materials, we determine which tensor components corresponds to the effective refractive indices by determining the direction of the Bloch mode’s dominant polarization.

You must either be clever in your choice of $\vec{\beta}$, or look at the polarization of the mode to determine which tensor element you are calculating.

\[
\begin{bmatrix}
  n_{\text{eff,1}} & 0 & 0 \\
  0 & n_{\text{eff,2}} & 0 \\
  0 & 0 & n_{\text{eff,3}}
\end{bmatrix}
\]

Procedure for Uniaxial Structures Using 2D PWEM

Step 1 -- Build the unit cell on grid.

Step 2 -- Define a single small Bloch wave vector in any direction.

\[ \hat{\beta} = 0.01\hat{\beta}_{\text{max}} \hat{x} \]

\( \beta_{\text{max}} = \pi/a \)

Only a single $\hat{\beta}$ is needed here.

Step 3 -- Calculate $n_{\text{o}}$ from the lowest-order eigen-value of the $H$ mode.

Step 4 -- Calculate $n_{\text{e}}$ from the lowest-order eigen-value of the $E$ mode.

Step 6 -- Assemble the tensor.

\[
\begin{bmatrix}
  n_{\text{o}} & 0 & 0 \\
  0 & n_{\text{e}} & 0 \\
  0 & 0 & n_{\text{e}}
\end{bmatrix}
\]

\[
\begin{bmatrix}
  \epsilon_{\text{o}} & 0 & 0 \\
  0 & \epsilon_{\text{e}} & 0 \\
  0 & 0 & \epsilon_{\text{e}}
\end{bmatrix}
\]

$\epsilon_{\text{o}} = n_{\text{o}}^2$

$\epsilon_{\text{e}} = n_{\text{e}}^2$
Refractive Index Retrieval Through Phase Response

Single-Pass Phase Vs. Device Phase

The single-pass phase is simply the phase a wave accumulates from one pass through the device. It does not include phase from interfaces or resonances.

The device phase is the overall phase change in a wave after reflection from, or transmitting through, a device. This accounts for phase from interfaces and resonance.
Single-Pass Phase Through a Slab of Material

The phase a wave accumulates by travelling a distance $d$ through a homogeneous material with refractive index $n$ is

$$\phi = 2\pi \cdot \frac{d}{\lambda} = 2\pi \cdot \frac{nd}{\lambda_0} = \frac{2\pi}{\lambda_0} nd = k_0 nd$$

The problem is that phase is bounded.

$$-\pi \leq \phi \leq \pi$$

So the measured or modeled phase is actually

$$\phi = k_0 nd + m(2\pi) \quad m = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

The integer $m$ is whatever value is necessary to make $-\pi < \phi < \pi$.

Slope of Phase Response

We can eliminate the troublesome $m(2\pi)$ term by differentiating the phase equation with respect to frequency or wavelength.

$$\phi = \frac{2\pi nd}{\lambda_0} + m(2\pi)$$

$$\frac{d\phi}{d\lambda_0} = \frac{2\pi nd}{\lambda_0^2}$$

We can now retrieve the refractive index from the slope of the phase response instead of the phase response directly.

No branching problems!! 😊
Now in Terms of Frequency

Transmission through a slab made of material with refractive index $n$ will produce a phase according to

\[ \phi = k_0 n d + m (2\pi) \]

where $k_0 = \frac{\omega}{c_0}$, $c_0$ is the speed of light, $\omega$ is the angular frequency, and $m$ is an integer.

The slope of this line is

\[ \frac{d\phi}{df} = \frac{2\pi nd}{c_0} \]

The effective refractive index is retrieved using

\[ n_{\text{eff}} = \frac{c_0}{2\pi \frac{d\phi}{df}} \]

Example #1: A Bragg Grating

- $\lambda_{\text{Bragg}} = 1550$ nm
- $n_1 = 1.50$
- $n_2 = 1.51$
- $d_1 = \frac{\lambda_{\text{Bragg}}}{4n_1} = 258.3$ nm
- $d_2 = \frac{\lambda_{\text{Bragg}}}{4n_2} = 256.6$ nm
- # Periods = 500
Example #1: Bragg Grating Response

Example #1: Unwrap Phase
Example #1: Compute $\frac{d\phi}{d\lambda}$

\[
\frac{d\phi}{d\lambda} \approx \frac{\phi(\lambda_{i+1}) - \phi(\lambda_{i-1})}{2\Delta\lambda}
\]

Example #1: Calculate $n_{\text{eff}}$ from $d\phi/d\lambda$

\[
n_{\text{eff}} = \frac{\lambda_0^2}{2\pi d} \frac{d\phi}{d\lambda_0}
\]
A Quick Study

**Baseline:** $n_1=1.5$, $n_2=1.51$, $\Delta n=0.01$, $\Delta \lambda=0$ nm, # periods=500

**Chirped:** $n_1=1.5$, $n_2=1.51$, $\Delta n=0.01$, $\Delta \lambda=10$ nm, # periods=500

**Higher $\Delta n$:** $n_1=1.5$, $n_2=1.52$, $\Delta n=0.02$, $\Delta \lambda=0$ nm, # periods=500

**More Periods:** $n_1=1.5$, $n_2=1.51$, $\Delta n=0.01$, $\Delta \lambda=0$ nm, # periods=5000

---

**Homogenization of Photonic Crystals**

The Problem (1 of 2)

Most homogenization deals with the situation where the unit cell is much smaller than the wavelength.

This is called the **long-wavelength limit**.

\[ \lambda_0 \gg a \quad \text{traditional metamaterials} \]

Most photonic crystals do not operate in the long wavelength limit.

\[ \lambda_0 \approx a \quad \text{most photonic crystals} \]

The Problem (2 of 2)

There is no choice of \([\mu]\) and \([\varepsilon]\) that can produce dispersion surfaces like this.

Photonic crystals usually involve physics that effective media cannot account for.

Effective properties of photonic crystals for short wavelengths is very limited and for specific cases only.

Very limited usefulness.
Kinematic Vs. Dynamic Properties

Reflection and Refraction

**Kinematic**
- How waves change direction at an interface
- Consequence of conservation of momentum
- Calculated by phase matching

**Dynamic**
- How waves change amplitude, phase, and polarization at an interface
- Consequence of continuity of the field
- Calculated through Fresnel equations

Three Methods for Determining Effective Refractive Index

- **Method 0** – Long-wavelength approach
  - Applies only highly subwavelength unit cells or sometimes when inclusions in a host medium are highly subwavelength.
- **Method 1** – Normal incidence method
- **Method 2** – Multiple-angle method
- **Method 3** – Bloch wave method
- **Method 4** – Dispersion surface method
Method 0 – Long-Wavelength Approach

In the long wavelength limit, effective refractive index is essentially just an average of the materials it is composed of.

\[
\frac{\varepsilon_{\text{eff}} - \varepsilon_{\text{host}}}{\varepsilon_{\text{eff}} + 2\varepsilon_{\text{host}}} = \sum_{i=1}^{N} f_i \frac{\varepsilon_i - \varepsilon_{\text{host}}}{\varepsilon_i + 2\varepsilon_{\text{host}}}
\]

Lorentz-Lorenz effective medium approximation.

\[
\sum_{i=1}^{N} f_i = 1
\]

The limits of \( \varepsilon_{\text{eff}} \) are set by the Weiner bounds.

Structure and anisotropy are not considered by this equation.

Method 1 – Normal Incidence Reflection and Transmission

This problem is the same as the Nicholson-Ross-Weir method.
Method 2 – Angle-Dependent Transmission and Reflection

More robust retrieval than single-angle method.


Method 3 – Bloch Wave Method (1 of 4)

The effective refractive index $n_{\text{eff}}$ of a Bloch wave can be estimated from a simulation by observing the wavelength $\lambda$.

$$n_{\text{eff}} = \frac{\lambda_0}{\lambda}$$

CAUTION: $n_{\text{eff}}$ is typically very sensitive to frequency and direction of propagation through the lattice. This limits the usefulness of the effective index model.

Method 3 – Bloch Wave Method (2 of 4)

Be careful. The field you are observing has the form
\[ \vec{E}(\vec{r}) = \vec{A}(\vec{r}) e^{-j\vec{\beta} \cdot \vec{r}} \]

Wavelength \( \lambda \) comes solely from \( \vec{\beta} \) and not from \( \vec{A}(\vec{r}) \).

\[ |\vec{\beta}| = \frac{2\pi}{\lambda} \]

Thus, you must ignore the fluctuations of the field arising from \( \vec{A}(\vec{r}) \) and observe only the planes of the Bloch wave due to \( \vec{\beta} \).

Method 3 – Bloch Wave Method (3 of 4)

For higher-order bands, it can be very difficult to determine the wavelength \( \lambda \) from a simulation. Notice that neither of the observed wavelengths \( S_L \) and \( S_H \) are equal to the actual wavelength \( \lambda \).

\[ S_L = \text{bright spot to bright spot} \]
\[ S_H = \text{bright spot to bright spot} \]
\[ S_L = \text{envelop peak to envelop peak} \]

\[ A(x, y) = A(x, y) e^{-j\beta x} \]

\[ e^{-j\beta x} \]

\[ 0 < a < 2a < 3a < 4a < 5a < 6a < 7a < 8a < 9a < 10a \]

\[ \text{Actual wavelength of Bloch wave} \]

\( S_L \) and \( S_H \) are actually sum and difference frequencies of \( a \) and \( \lambda \).

\[ \frac{1}{S_L} = \frac{1}{a} - \frac{1}{\lambda} \]
\[ \frac{1}{S_H} = \frac{1}{a} + \frac{1}{\lambda} \]
Example
In practice, we only ever observe \( A(x,y) e^{j\beta x} \).

From this we read off...

\[ S_L \approx 3.00a \quad S_H \approx 0.43a \]

We solve our sum and difference frequency equations for \( \lambda \).

\[
\begin{align*}
\frac{1}{2} + \frac{1}{a} S_a - \frac{1}{a} S \lambda &= \frac{4}{3a} \quad \Rightarrow \lambda = \frac{3a}{4} = 0.75a \\
\frac{1}{a} S_a - \frac{1}{a} S \lambda &= 0.43a - \frac{1}{a} a = 0.57 \quad \Rightarrow \lambda = 0.43a - 0.57 \\
\frac{2}{2} + \frac{1}{a} S_a - \frac{1}{a} S \lambda &= \frac{1}{3a} + \frac{1}{a} 1.29a \quad \Rightarrow \lambda = \frac{1.29a}{3.43} = 0.75a \\
\end{align*}
\]

Proof / Derivation

\( A(x,y) e^{j\beta x} \rightarrow \cos \left( \frac{2\pi}{a} \right) \cos \left( \frac{2\pi}{a} \right) \)

\[ \frac{1}{2} \cos \left( \frac{2\pi}{a} \right) \frac{2\pi}{a} \right) \frac{1}{2} \cos \left( \frac{2\pi}{a} \right) \frac{2\pi}{a} \right) \]

Average \( \lambda \)

\[
\begin{align*}
\frac{1}{a} S_a - \frac{1}{a} S \lambda &= 0.43a - 0.57 \\
\frac{2}{2} + \frac{1}{a} S_a - \frac{1}{a} S \lambda &= \frac{1}{3a} + \frac{1}{a} 1.29a \quad \Rightarrow \lambda = \frac{1.29a}{3.43} = 0.75a \\
\end{align*}
\]

Method 4 – Dispersion Surfaces

Calculating Phase Refractive Index

Step 1 – Define \( \vec{\beta} \)

Step 2 – Calculate eigen-frequency (i.e. wave number \( k_0(\vec{\beta}) \)).

Step 3 – Calculate effective index.

\[ n_{EFS} = \left| \frac{\vec{\beta}}{k_0(\vec{\beta})} \right| \]

Note: this is a phase refractive index.
If a metamaterial can be replaced by a homogeneous material and it behaves the same way, the homogeneous material has the effective material properties of the metamaterial.
Parameter Retrieval

Parameter retrieval is the process whereby we calculate the effective material properties.

This is ding dang hard!!!
S-Parameters from a VNA

The scattering parameters are complex quantities because they modify amplitude and phase of a wave. They can be expressed in either rectangular or polar coordinates.

\[
S = S' + jS'' = \left| S \right| \angle S
\]

Vector network analyzers typically report the scattering parameters in terms of magnitude and phase, where the magnitude is given as a power quantity in decibels and the phase in degrees.

\[
S_{\text{magnitude}} = 10 \log_{10} \left( |S|^2 \right) = 20 \log_{10} \left( |S| \right)
\]

\[
S_{\text{phase}} = \angle S
\]