Homogenization of layered media: Intrinsic and extrinsic symmetry breaking

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Abstract – A general homogenization procedure for periodic electromagnetic structures, when applied to layered media with asymmetric lattice cells, yields an effective tensor with magnetoelectric coupling. Accurate results for transmission and reflection are obtained even in cases where classical effective medium theory breaks down. Magnetoelectric coupling accounts for symmetry breaking in reflection and transmission when a non-symmetric structure is illuminated from two opposite sides.

Introduction. – A useful way to understand the properties of a periodic photonic heterostructure, such as a metamaterial or photonic crystal, is to represent it as a homogeneous effective medium. Effective medium descriptions are known to be accurate in the long-wavelength limit $a/\lambda \rightarrow 0$, where $a$ is the unit cell size and $\lambda = 2\pi c/\omega$ is the free-space wavelength, but break down when $a/\lambda$ becomes appreciable [1–6]. A qualitative manifestation of this breakdown occurs when there are incompatible symmetries between the scattering characteristics of the original heterostructure and the respective homogenized sample.

As an example, consider wave propagation in a dielectric multilayer consisting of repeated layers labeled $\alpha$ and $\beta$, surrounded by air, as shown in fig. 1(a). The layers have unequal dielectric constants $\epsilon_\alpha$ and $\epsilon_\beta$ (which may be complex and dependent on the frequency $\omega$), so that the heterostructure lacks mirror symmetry with respect to the normal direction $n$. In fig. 1(b), the solid lines show the phases of the reflection coefficients $R_{\alpha\beta}$ and $R_{\beta\alpha}$, calculated analytically using the transfer matrix technique [7], for $s$-polarized waves impinging normally on the structure with $\alpha \beta \ldots$ and $\beta \alpha \ldots$ layer orderings, respectively. (Reflection coefficients are the ratios of the complex amplitudes of the electric field in the reflected and incident waves.) In the static limit $a/\lambda \rightarrow 0$, the order of the layers is unimportant, but for larger values of $a/\lambda$ the phases differ substantially [3–5,8]. We call this effect, which arises from the lack of mirror symmetry of the underlying heterostructure, intrinsic symmetry breaking (ISB).

A related but different effect, which we call extrinsic symmetry breaking (ESB), manifests itself when the external media on the two sides of the structure are different. In that case, not only the phases but also the magnitudes of the reflection coefficients may differ [3]. When the medium on one side is optically denser than the static average in the slab, different layer orderings can produce extremely different reflection coefficients when the incident wave is close to the critical angle for total internal reflection. (This phenomenon does not contradict optical reciprocity [9].)

Symmetry breaking and homogenization. – At first glance, it seems that ISB cannot be faithfully reproduced by a homogenized slab, since a homogeneous medium would have an inherent mirror symmetry ensuring that $R_{\alpha\beta} = R_{\beta\alpha}$. For instance, for $s$-waves and equal layer widths, standard quasi-static homogenization leads to a simple dielectric structure with the scalar effective permittivity $\epsilon_{\text{eff}} = (\epsilon_\alpha + \epsilon_\beta)/2$. Obviously, no symmetry breaking can occur in this case.

In the metamaterials literature, it is common to consider nonlocal homogenization (non-pointwise constitutive
relations between the fields) [1,2,6,10,11]; equivalently, effective material parameters depend on the Fourier-space wave vector $k$. In these nonlocal theories, the $k$ vector is considered as arbitrary, which amounts to having infinitely many degrees of freedom by which transmission and reflection of waves can be fitted. Even then, additional augmentations to the model are necessary to account for ISB. For example, Lei et al. introduced an artificial matched layer on the illumination side [8]. However, this is not satisfactory, since an effective medium ought to reflect the intrinsic characteristics of the structure, independent of the illumination conditions. In particular, if the layered slab is illuminated from both sides, then two artificial layers would have to be introduced, and their matching properties would be frustrated due to the coupling between those layers.

In sharp contrast, we show here that an appropriate local homogenization scheme can accurately account for ISB via magnetoelectric (ME) couplings in the effective material tensor. No artificial matching layers, auxiliary boundary conditions or complicated non-local formulations are required. Details about the homogenization scheme are given below; when applied to the above multilayer structure, it produces the values plotted as markers in fig. 1(b), which are in excellent agreement with the exact transfer matrix results. In particular, arg($R_{\alpha\beta}$) = arg($R_{\beta\alpha}$) in the $a/\lambda \to 0$ limit, but these values differ for shorter wavelengths, so that ISB is quantitatively accounted for.

**Linear constitutive relations and magnetoelectric coupling.**

*General considerations.* In their most general form, local linear constitutive relations couple one pair of electric and magnetic fields to the other pair. For example, the $\mathbf{D}, \mathbf{H}$ fields could be expressed as linear combinations of $\mathbf{E}$ and $\mathbf{B}$ [12–14]. Equivalently, by a linear transformation, one can write the $\mathbf{E}, \mathbf{H}$ pair in terms of $\mathbf{D}, \mathbf{B}$ (e.g., [15]) or, alternatively, $\mathbf{D}, \mathbf{B}$ via $\mathbf{E}, \mathbf{H}$ [16,17].

The most general bi-anisotropic relations, with their related controversies (non-reciprocity, the Post constraint) [13–15] are outside the scope of this letter. Rather, we focus on the particular case of s-waves propagating through a material slab (although p-polarization could be handled in a similar way). The 3-vector $(\mathbf{D}, \mathbf{B}_n, \mathbf{B}_\tau)$ gets expressed via the 3-vector $(\mathbf{E}, \mathbf{H}_n, \mathbf{H}_\tau)$; in general, this relationship couples electric and magnetic fields, as discussed in more detail below.

*Magnetoelectric coupling for s-polarization.* To elucidate the origin of ME coupling, we first consider the simple case of an isotropic lossless homogeneous medium with two s-polarized plane waves propagating in opposite axial directions $\pm n$, indicated in fig. 1(a). The respective equal-magnitude wave vectors are $\pm \mathbf{q} = \pm Q \hat{q}$, where $Q$ is the wave number in the medium and $\hat{q}$ is a unit vector; the respective electric and magnetic field components are

$$E_z^\pm = E_0^\pm \exp(\pm iq \cdot \mathbf{r}), \quad H_\tau^\pm = H_0^\pm \exp(\pm iq \cdot \mathbf{r}) \tag{1}$$

where $\mathbf{r} = (n, \tau, z)$. The waves satisfy Maxwell’s equations

$$\nabla \times \mathbf{E} = ik_0 \mathbf{B}, \quad \nabla \times \mathbf{H} = -ik_0 \mathbf{D} \tag{2}$$

under the exp($-i\omega t$) phasor convention. The medium is described by a material tensor $\mathcal{M}$ whose matrix representation $M$ in a given coordinate system satisfies

$$\Psi_{DB} = M \Psi_{EH}, \quad \Psi_{DB} = \begin{bmatrix} D_{0z}^+ & D_{0z}^- \vspace{1mm} \noalign{
\phantom{\Psi_{DB}} = \begin{bmatrix} \noalign{\phantom{\Psi_{DB}}}} B_{0\tau}^- & B_{0\tau}^+ \end{bmatrix} \end{bmatrix}, \quad \Psi_{EH} = \begin{bmatrix} E_{0z}^- & E_{0z}^+ \vspace{1mm} \noalign{\phantom{\Psi_{DB}} = \begin{bmatrix} \noalign{\phantom{\Psi_{DB}}}} H_{0\tau}^- & H_{0\tau}^+ \end{bmatrix} \end{bmatrix} \tag{3}$$

Normalizing the $E_{0z}$ amplitudes to unity and applying Maxwell’s equations gives

$$\Psi_{DB} = q \begin{bmatrix} -Y_+ & Y_- \vspace{1mm} \noalign{\phantom{\Psi_{DB}} = \begin{bmatrix} \noalign{\phantom{\Psi_{DB}}}} 1 & 1 \end{bmatrix} \end{bmatrix}, \quad \Psi_{EH} = \begin{bmatrix} 1 & 1 \vspace{1mm} \noalign{\phantom{\Psi_{DB}} = \begin{bmatrix} \noalign{\phantom{\Psi_{DB}}}} Y_+ & Y_- \end{bmatrix} \end{bmatrix} \tag{4}$$

where $Y_{\pm} = H_{0\tau}^\pm / E_{0z}^\pm$ are the wave admittances. Then

$$M = \Psi_{EH}^{-1} \Psi_{DB} = \frac{q}{Y_2 - Y_1} \begin{bmatrix} -2Y_1 Y_2 \vspace{1mm} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = } = \begin{bmatrix} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = }} Y_1 + Y_2 \end{bmatrix} \end{bmatrix} Y_1 + Y_2 \vspace{1mm} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = } = \begin{bmatrix} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = }} 2 \end{bmatrix} \end{bmatrix}, \quad \begin{bmatrix} D_z \\ B_\tau \end{bmatrix} = M \begin{bmatrix} E_z \\ H_\tau \end{bmatrix} \tag{5}$$

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$$M = \Psi_{EH}^{-1} \Psi_{DB} = \frac{q}{Y_2 - Y_1} \begin{bmatrix} -2Y_1 Y_2 \vspace{1mm} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = } = \begin{bmatrix} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = }} Y_1 + Y_2 \end{bmatrix} \end{bmatrix} Y_1 + Y_2 \vspace{1mm} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = } = \begin{bmatrix} \noalign{\phantom{M = \Psi_{EH}^{-1} \Psi_{DB} = }} 2 \end{bmatrix} \end{bmatrix}, \quad \begin{bmatrix} D_z \\ B_\tau \end{bmatrix} = M \begin{bmatrix} E_z \\ H_\tau \end{bmatrix} \tag{7}$$
The ME coupling is represented by the off-diagonal terms in $M$, and is absent if and only if $Y_1 = -Y_2$, which is the case for an ordinary homogeneous dielectric medium.

In a periodic medium, the two plane waves (1) are replaced with Bloch waves, and $Y_{1,2}$ are the boundary admittances of these Bloch waves. We conclude from (6) that ME coupling arises whenever these boundary admittances are different, which in general is indeed the case for non-symmetric structures.

Note that this type of ME coupling is not equivalent to optical activity. It does not alter the polarization of the wave, which remains $s$-polarized throughout. By contrast, the constitutive relations for optically active media typically include a contribution to $D$ in the direction of $B$, as well as a contribution to $B$ in the direction of $E$ [12,18,19].

Homogenization procedure. – We now adopt the homogenization scheme described in [20,21], which generates an effective tensor $\mathcal{M}$ for a layered heterostructure by approximating the fields on two scales, one finer and the other one coarser than the lattice cell size. The fine-scale fields are approximated by a basis set of Bloch waves traveling in different directions. The coarse-scale basis consists of the respective generalized plane waves, which must satisfy i) Maxwell’s equations within the sample and ii) Maxwell’s boundary conditions for the tangential components of the electric and magnetic fields on the boundary of the sample.

To satisfy ii), the plane wave amplitudes are computed as boundary averages of the periodic factors of Bloch waves; to satisfy i), the $\Psi_{DB}$ and $\Psi_{EH}$ matrices are rectangular, with the number of columns equal to the number of basis functions. Hence (3) is in general interpreted in the least squares sense rather than an exact equality; see [20,21] for further details.

Intrinsic symmetry breaking: analytical insight. – We apply this procedure to $s$-polarized waves in the multilayer heterostructure of fig. 1(a) (the $p$-wave case can be dealt with similarly). To get an analytical insight, we again take all the materials to be lossless, so that $\epsilon_\alpha$ and $\epsilon_\beta$ are real, and consider a fine-scale basis of only two Bloch waves propagating in the normal direction $n$, with their Bloch wave numbers $\pm q$ at the operating frequency:

$$e_1(n) = u(n) \exp(iqn), \quad h_1(n) = -k_0^{-1}[q u(n) - i u'(n)] \exp(iqn),$$

$$e_2(n) = u'(n) \exp(-iqn), \quad h_2(n) = k_0^{-1}[q u'(n) + i u''(n)] \exp(-iqn).$$

Here $u(n)$ denotes the lattice-periodic factor for the electric field, and $\cdot'$ indicates complex conjugates. On the coarse scale, our procedure defines the $EH$ amplitudes of plane waves as the boundary values ($n = 0$) of theBloch waves:

$$E_{0z}^+ = u(0), \quad H_{0r}^+ = -k_0^{-1}[q E_0^+ - i u'(0)],$$

$$E_{0z}^- = u^*(0), \quad H_{0\gamma}^- = k_0^{-1}[q E_0^- + i u''(0)].$$

The corresponding admittances are therefore

$$Y_1 = -k_0^{-1}[q - i \epsilon_1'(0)/\epsilon_1(0)], \quad Y_2 = k_0^{-1}[q + i \epsilon_1''(0)/\epsilon_1'(0)].$$

An explicit expression for the ME coupling term is

$$M_{12} = \frac{q}{k_0} \frac{\text{Re} \eta}{\text{Im} \eta + q}, \quad \eta \equiv \frac{u'(0)}{u(0)}$$

Hence the ME coupling arises from the difference in the boundary admittances of the Bloch waves. If the lattice cell possesses mirror symmetry, then the derivative $u'(0)$ vanishes, so $M_{12} = 0$.

Importantly, the matrix representation of $M$ depends on the choice of coordinate system. If $(n, \tau, z)$ is switched to the mirror-image system $(n', \tau', z)$ shown in fig. 1(a), the off-diagonal ME terms reverse sign. The effective medium is thus able to capture the effects of the broken mirror symmetry, as demonstrated by the numerical results of fig. 1(b).

Example: local homogenization and intrinsic symmetry breaking. – Turning now to ESB effects, we set the same parameters as in [3]: equal layer widths $d_\alpha = d_\beta = a/2 = 10\text{nm}$, dielectric constants $\epsilon_\alpha = 5$ and $\epsilon_\beta = 1$, and free-space wavelength $\lambda = 500\text{nm}$. The effective permittivity for the $s$ mode in the static limit $(a/\lambda \to 0)$ is $\epsilon_{\text{stat}} = (\epsilon_\alpha d_\alpha + \epsilon_\beta d_\beta)/a = 3$. The number of lattice cells $N$ is allowed to vary. External dielectric permittivities are $\epsilon_{\text{in}} = 4$ and $\epsilon_{\text{out}} = 3$ on the sides of incidence and transmission, respectively. These parameters match the ones of [3] and, since $\epsilon_{\text{in}} \neq \epsilon_{\text{out}}$, give rise to ESB. In the static limit, the critical angle for total internal reflection is

$$\theta_{\text{crit}} = \sin^{-1} \sqrt{\epsilon_{\text{stat}}/\epsilon_{\text{in}}} = 60^\circ.$$  

Once the angle of incidence reaches the critical value, the wave in the $\beta$ layer becomes evanescent, but the wave in the $\alpha$ layer is propagating.

For this setup, the fine-scale basis in our homogenization procedure contains Bloch waves with the tangential components of the Bloch wave vector $q_r = m \epsilon_{\text{stat}} k_0/(m_q - 1)$, where $0 \leq m < m_q$, and $m_q$ is a parameter defined below. Only non-negative values of $q_r$ are needed due to the symmetry of the structure in the tangential direction. For each $q_r$, there are two Bloch waves in the forward and backward directions; hence the total size of the Bloch basis is $2m_q$.

On the coarse level, the basis consists of the respective $2m_q$ generalized plane waves. We will take $m_q = 7$; the results shown below are essentially unchanged for other choices of $m_q \geq 5$. 

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Near $\theta_{\text{crit}}$, the reflection and transmission coefficients are found to depend strongly on the choice of layer order ($\alpha\beta\ldots$ or $\beta\alpha\ldots$), and both are very different from the values predicted by the static permittivity $\epsilon_{\text{stat}}$; see [3] and fig. 2. Plots in fig. 2 show the reflectance and the phase of the reflection coefficient against the number of lattice periods $N$ in the slab. (Since each until cell has two layers, the total number of layers is $2N$.) To our knowledge, no published homogenization procedures are capable of accurately reproducing transmission and reflection from asymmetric structures, unless an auxiliary artificial layer is introduced, as done by Lei et al. [8]. (As already noted, such a layer does not represent intrinsic characteristics of the structure and is good for one-sided illumination only.)

In fig. 2 we compare our homogenization results with both classical quasi-static (QS) homogenization and the popular “current-driven” (CD) homogenization scheme [10] without artificial matching layers. (Implementation of CD homogenization is described in detail in [22].)

It is clear that the QS and CD results are qualitatively inaccurate in this case. This is not surprising because, among other things, QS and CD models do not include a mechanism for representing ISB; in particular, $R_{\text{CD}} = R_{\text{CD,ab}} = R_{\text{CD,ba}}$, unless artificial boundary layers are introduced. Moreover, the detailed analysis and simulations of [22] led to the conclusion that, overall, CD homogenization “does not yield accurate results in the range of parameters where it predicts nontrivial magnetic effects”, although slight improvements in the accuracy of the $T$ coefficient were noted in some narrow parameter ranges. A separate and independent study [23] concluded, in agreement with [22], that “the permeability obtained from current-driven homogenization is useless in predicting reflection from a 1D layered structure” (but improvement was observed in the case of reflection from semi-infinite 2D resonating structures at long wavelengths [23]).

In contrast, our homogenization produces magnetoelectric coupling automatically and yields TR coefficients agreeing extremely well with the exact results obtained by transfer matrix calculations (fig. 2). More specifically, figs. 3(a), (b) show that the relative errors in the reflection coefficients $R_{\alpha\beta}, R_{\beta\alpha}$ are at least two orders of magnitude lower than in static or CD homogenization.
Our homogenization captures the substantial differences between the $\alpha\beta\ldots$ and $\beta\alpha\ldots$ layer orderings [3] via the ME coupling in the $\mathcal{M}$ tensor. For instance, 

\[
M(a/\lambda = 0.04) \approx \begin{bmatrix}
3.02 & 0 & -0.128i \\
0 & 1 & 0 \\
0.128i & 0 & 1
\end{bmatrix}, \quad (18)
\]

or more explicitly $D_z \approx 3.02E_z - 0.128i H_z$; $B_n \approx H_n$; $B_\tau \approx 0.128iE_z + H_z$. The effective permittivity differs slightly from its static value of 3, but the key feature is the presence of the ME coupling terms, which are clearly appreciable. The magnitude of the ME coupling is approximately proportional to $a/\lambda$ and vanishes in the static limit $a/\lambda \to 0$, as shown in fig. 3(c).

**Conclusion.** – We have demonstrated that our homogenization procedure [20,21], which automatically produces an effective material tensor with magnetoelectric coupling terms, can accurately describe the behavior of periodic multilayer heterostructures away from the static limit. The general features of this procedure are as follows:

1) The effective material tensor is independent of the illumination conditions.

2) The effective tensor automatically accounts for anisotropy, magnetic response and magnetoelectric coupling.

3) Intrinsic and extrinsic symmetry breaking are rendered accurately. No artificial boundary layers, non-local effects or other amendments are employed.

In contrast, to the best of our knowledge, in the existing publications the only way to account for ISB is via an artificial matching layer introduced on the boundary of the sample. Such a layer is extrinsic to the sample and works only for one-sided illumination. If a layered slab is illuminated from both sides, then two artificial layers would need to be introduced; however, the coupling between them will debilitate the matching (not to mention possible extensions of the theory to 2D and 3D samples finite in all coordinate directions).

Any local homogenization will break down once the wavelength becomes sufficiently short. The accuracy of our procedure at short wavelengths was examined in prior publications [20,21]; this accuracy is significantly improved in the non-local version of our method [21]. However, these issues do not arise in the current letter, since its subject is symmetry breaking at long wavelengths.

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