Group theoretical description of artificial magnetic metamaterials utilized for negative index of refraction

W. J. Padilla
Los Alamos National Laboratory, MS G756, MST-CINT, Los Alamos, NM 87545.

Group theoretical methods are used to determine the electromagnetic properties of artificial magnetic meta-materials, based solely upon the symmetries of the underlying constituent particles. Point groups for such materials are determined. From the transformation properties of an electromagnetic (EM) basis under symmetries of the particles, it is possible to determine, (i) the EM modes of the particles, (ii) the form of constitutive relations (iii) magneto-optical response of a meta-material or lack thereof. These methods are shown to be useful for determination of the isotropic or bi-anisotropic nature of artificial magnetic particles. The results for several artificial magnetic metamaterials are given. Based upon these methods, we predict an ideal planar artificial meta-material, which eliminates an undesirable electric resonance while still exhibiting a magnetic response. Further we determine the subset of point groups of which particles must belong to in order to yield an isotropic 3D magnetic response, and we show an example.

Progress in the rapidly advancing field of metamaterials has experienced even further growth due to the recent observation of a negative index (NI) medium. A NI medium is an artificial material in which both the magnetic $\mu$ and electric $\varepsilon$ response obtain simultaneous negative values, thus yielding a negative index of refraction. Although predicted over three decades ago, it wasn’t until recently that such materials were realized. Typically NI media utilize individual components for the electric and magnetic response. Materials which exhibited negative epsilon, known as artificial dielectrics, have been known since the 40’s. The critical component responsible for the demonstration of NI was the realization that artificial non-magnetic materials could be constructed to exhibit negative response.

The first demonstrations of NI materials were performed at microwave frequencies, due in part to the ease of fabrication as well as simplicity of measurements. The magnetic component of NI materials have since been demonstrated at lower RF frequencies and higher THz frequencies. Great interest for the further extension of these exotic materials to optical frequencies (utilizing nano-sized elements) is fuelling massive research efforts. Given the potential of NI materials to span the electromagnetic spectrum, it is important to understand their full complex electromagnetic behavior. In particular, the structures utilized for NI are bianisotropic and may yield rich electromagnetic properties such as chirality $\kappa$ and/or non-reciprocity $\chi$.

At microwave frequencies where complex reflection and transmission measurements (S-parameter) are common, it is difficult to characterize bianisotropic materials. This difficulty stems from the fact that these materials are necessarily described by the most general form of the constitutive relations. There may be 36 complex quantities to determine, and thus standard complex reflection and transmission measurements yield incomplete EM information. At THz and higher frequencies where phase sensitive measurements are not common it is even more difficult, although methods such as ellipsometry or THz time domain spectroscopy may prove useful. Further since a magnetic and electric resonant response enter similarly into the Fresnel equations, it is difficult to determine the origin of the response. Typically, artificial magnetic metamaterials are constructed from conducting elements, and thus a full electromagnetic characterization is a necessity, since an electric response is unavoidable. Analytical theories have yielded equations able to predict the resonant frequency $\omega_0$ and plasma frequency $\omega_p$ of metamaterials. However there is a lack of suitable analytical methods capable of determining the many varying and complicated EM properties. Simulation is still heavily relied upon and, as of yet, is still unable to determine and distinguishing bianisotropic response.

We present a group theoretical method capable of determining various electromagnetic properties for magnetic metamaterials. This method is based simply upon the symmetry operations of the constituent particles about a point in space, i.e. point group theory. An EM basis is assigned to the artificial particle under investigation, and transformations of this basis under the symmetries of the group yield the electromagnetic modes. This new method allows one to calculate: the EM modes, the form of the constitutive relations, and the determine whether a particle will exhibit magneto-optical response. This approach is demonstrated by way of an example.

Materials utilized for negative magnetic response have been shown to be bianisotropic, thus let us review the constitutive relations for these materials, which can be written as:

$$
\begin{bmatrix}
\mathcal{E} \\
\mathcal{B}
\end{bmatrix} =
\begin{bmatrix}
\xi & \eta \\
\xi & \eta
\end{bmatrix}
\begin{bmatrix}
\mathcal{E} \\
\mathcal{B}
\end{bmatrix}
$$

(1)

In Eq. (1) the permittivities within the 2x2 matrix are tensors of second rank, also called dyadics. The terms $\xi$ and $\eta$ are called the magneto-optical permittivities,
and they describe coupling of the magnetic to electric response and electric to magnetic response respectively.

As an example, let us start by examining the point group symmetries of a typical element utilized for magnetic response. In Fig. 1(b-d) the symmetry operations of a split ring resonator (SRR) are shown. A symmetry operation brings the element into self coincidence. Thus for the SRR it can be seen that there are three symmetries which meet this criterion. In addition, all groups also contain the identity operation E. We then find that the SRR particle belongs to the $C_{2v}$ point group which contains the following elements $[E, c_2, \sigma(xy), \sigma(xz)]$ where we use the Schoenflies notation.

We now turn to determination of the EM modes of the particles. Since we have determined SRRs to belong to the $C_{2v}$ group we can utilize the character table for this analysis (see Table I). With the character table we can assign a basis set to the SRR and see how this basis set transforms under the symmetry operations of the SRR. For brevity we only consider the outer split ring, however the inner ring is also easily handled by this method. We want our basis to represent areas of electrical activity, thus we choose the basis shown in the left column of Fig. 2(b). Regions marked with arrows represent areas which can be polarized by an external electric field (i.e. currents can flow in these directions). These are similar to the $P$ orbitals used in molecular orbital group theory (MOGT). The next step is to write out matrices which describe how this basis transforms under $C_{2v}$. For example, there are five vectors which make up our basis for the SRR, and since the identity leaves the particle unchanged, this would be a 5x5 matrix with 1’s along the diagonal. Once we obtain matrix representations for each element of the group, we can use a result of the Orthogonality Theorem to determine how many times each irreducible representation (irrep) occurs. For our chosen basis we use the following equation:

$$a_m = \frac{1}{h} \sum_c n_c \chi(g) \chi_m(g)$$  \hspace{1cm} (2)

where $h$ is the order of the group ($h=4$ in this case), $n_c$ is the number of symmetry operation in each class, $\chi(g)$ are the characters of the original representation, and $\chi_m$ are the characters of the $m^{th}$ irreducible representation. Using Equation (2) we find our basis is spanned by $\Gamma_{SRR} = 2A_1 + 3B_2$.

| $C_{2v}$ | E $C_2$ $\sigma(xz)$ $\sigma(xy)$ | Linear | Quadratic |
|----------|---------------------------------|--------|-----------|
| $A_1$    | 1 1 1 1                          | x      | $x^2, y^2, z^2$ |
| $A_2$    | 1 1 -1 -1                        | $R_x$  | $yz$      |
| $B_1$    | 1 -1 1 -1                        | $z, R_y$ | $xz$    |
| $B_2$    | 1 -1 -1 1                        | $y, R_z$ | $xy$    |
| $\Gamma_{SRR}$ | 5 -1 -1 1 | 5      |           |

Once we know the irreps spanned by an arbitrary basis set, we can work out the appropriate linear combinations of basis functions that transform the matrix representations of our original representation into block diagonal form. These are called symmetry adapted linear combinations (SALCs). We use a projection operator to determine the SALCs, that transforms as an irrep. This is given by,

$$\phi'_i = \frac{1}{\sqrt{c_k}} \sum_g \chi_k(g) g \phi_i$$  \hspace{1cm} (3)

where $\phi'_i$ is the SALC, $\chi_k$ is the character of the $k^{th}$ irrep, $g$ is the symmetry operation, and $\phi_i$ is the basis function.

We can normalize the SALCs determined by Equation (3), but this is not necessary since a constant factor doesn’t affect the symmetry of the calculated modes. The response of the SRRs can now be determined by considering incident external electromagnetic fields. For example by examination of the character table for the $C_{2v}$ point group we see that light polarized along the $\hat{x}$-axis transforms as $A_1$, since it transforms in the same manner as

FIG. 1: Point group symmetries of the SRR particle. Panel (a) shows the coordinate system convention. Panel (b) shows the symmetry axis of the SRR and the $C_2$ symmetry (rotation about the axis by $2\pi/n$, $n=2$). Panels (c) and (d) demonstrate the mirror plane symmetries.
the function $x$. Thus $\hat{y}$-polarized light transforms as $B_2$ symmetry. The function $R_\alpha$ represents rotation about the $\alpha$ axis, where $\alpha=\hat{x}, \hat{y}, \hat{z}$. Thus a magnetic field polarized along the $\hat{z}$-direction also transforms as $B_2$ symmetry. We summarize these results in Fig. 2 for: (a) planar spirals, (b) SRRs, (c) Omega particles, (d) an SRR and its enantiomer, (e) symmetric ring resonator.

An electric field polarized along the $\hat{x}$-axis ($A_1$) of the SRR drives currents as shown in row (b) of Fig. 2. This would give a frequency response determined by the dimensions (length) of the SRR segments along which $E_x$ lies. For $\hat{y}$-polarized ($B_2$) light much more exotic behavior is predicted. Notice that for the irrep of $B_2$ both $y$ and $R_z$ form a suitable basis. Thus we can use a linear combination of these two functions for the basis. This predicts that the SRR should exhibit a magneto-optical response, as in accord with MOGT. Furthermore, since $E_y$ and $B_z$ are the same basis, they will occur at the same frequency. In other words, an $E$ field polarized along the $\hat{y}$-axis will result in a resonant response at a frequency $\omega_0$, and a magnetic field polarized along the $\hat{z}$-axis will result in a resonant response at the same frequency $\omega_0$. These theoretical predictions are consistent with results obtained from a simple analytical model as well as by simulation.

In Fig. 2 we show predictions for other various magnetic metamaterials. Particles with the lowest symmetry are listed on the top and higher symmetry particles on the bottom. The artificial magnetic metamaterials listed in the first 3 rows are shown to be bianisotropic, and thus we list the form of the constitutive equations governing the predicted magneto-optical response on the right side of each row. In row (d) we show a particular way of symmetrizing the SRR particle, which we predict will eliminate the magneto-optical response. The material is a bipartite lattice with each of the two sub-lattices consist-

FIG. 2: Basis utilized (red arrows in left column) for magnetic metamaterials used to calculate the EM modes (red arrows in the remaining columns). The remaining columns for each row show the SALCs and modes of the SRR particle, as determined by point group symmetries. For each column, the irrep is shown above and the corresponding component of the an external electromagnetic wave, or function is shown.
ing of SRRs each with the gap oriented oppositely. Thus it is predicted that any polarization rotation or mixing resulting from one unit cell is corrected by the other unit cell, resulting in no net polarization rotation. Indeed it can be seen that the theory predicts no magneto-optical activity, while still exhibiting a magnetic response for $B_z$.

Another predicted way to eliminate $\xi$ and $\zeta$ is to add a second gap in the SRR opposite to the first, as shown in Fig. 2(e). Again the theory predicts no magneto-optical response and thus we have eliminated bianisotropy by symmetrizing the SRR. This structure is simpler than that depicted in Fig. 2(d) and we have a predicted magnetic response for $B_z$.

Lastly let us turn to the prediction of an ideal magnetic metamaterial. With our new understanding of the irreps of a point group and their relation to magneto-optical behavior we can leverage point group tables for help. An ideal magnetic particle is one in which no magneto optical behavior is predicted. In the parlance of group theory this implies we should look for a point group which has linear basis functions with rotational functions $R_\alpha$ but with little or no occurrences of linear $\hat{x}, \hat{y}, \hat{z}$ functions. This not only ensures the elimination of the $\xi$ and $\zeta$ terms, but also off-diagonal terms in the $\mu$ and $\epsilon$ response functions, like those which occur for the particle listed in Fig. 2(d), i.e. $3B_g$ and $2B_u$. In Table II we show a candidate point group which should have good magnetic response with no magneto-optical activity, and no frequency dependent $\epsilon$ occurring near the magnetic resonance. A particle which has the symmetry of this group is shown in Fig. 3.

Group theoretical analysis is carried out for the particle depicted in Fig. 3(a), and we find the following modes $\Gamma=A_{1g}+A_{2g}+ B_{1g}+B_{2g}+ 2E_u$. Thus the only linear modes determined are a magnetic mode ($A_{2g}$) and an electric mode ($E_u$). The fact that the electric mode does not occur in the same irrep as the magnetic mode ensures it will not occur at the same frequency. Further the two dimensional $E_u$ mode implies the electric response of the particle will be identical along the $\hat{x}$ and $\hat{y}$ directions with no cross coupling terms ($\epsilon_{xy}=\epsilon_{yx}=0$). Thus if we want to construct a 3D isotropic magnetic metamaterial free from magneto-optical activity, then the geometry of the constituent particles are required to be one of the following point groups: $T_h, T_d, I_h$, and $O_h$. The two simplest of which to visualize is $I_h$, an icosahedron, and $O_h$, a cube (depicted in Fig. 3(b)) or octahedron.

We have demonstrated a new method capable of determining various properties of the electromagnetic response for artificial magnetic metamaterials. A specific example has been worked out for the most common element utilized for negative magnetic response. This analysis has also been carried out and detailed for other various artificial magnetic metamaterials. We have predicted 2 ideal magnetic particles, including one for 3D isotropic magnetic response. Whether one wants to take advantage of the exotic electromagnetic properties that emerge from the bianisotropic nature of artificial metamaterials, or construct artificial materials free from this complication, these novel methods are valuable for determining the expected response.

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**TABLE II: Character table for the D_{4h} point group.**

| $\text{D}_{4h}$ | $E$ | $2C_{4}(z)$ | $C_{2}$ | $2C'_{2}$ | $2C''_{2}$ | $i$ | $2S_{4}$ | $\sigma_{h}$ | $2\sigma_{v}$ | $2\sigma_{d}$ | Linear |
|----------------|------|-------------|--------|-----------|----------|-----|--------|------------|----------|------------|--------|
| $A_{1g}$       | 1    | 1           | 1      | 1         | 1        | 1   | 1      | 1          | 1        | 1          | 1      |
| $A_{2g}$       | 1    | 1           | -1     | -1        | 1        | 1   | -1     | -1         | 1        | -1         | 1      |
| $B_{1g}$       | 1    | -1          | 1      | -1        | 1        | 1   | -1     | -1         | 1        | -1         | 1      |
| $B_{2g}$       | 1    | -1          | -1     | 1         | -1       | 1   | 1      | 1          | -1       | 1          | -1     |
| $E_{g}$        | 2    | 0           | -2     | 0         | 0        | 2   | 0      | -2         | 0        | 0          | 2      |
| $E_{u}$        | 2    | 0           | -2     | 0         | 0        | -2  | 0      | 2          | 0        | 0          | 2      |

**FIG. 3:** Predicted ideal planar and ideal 3D magnetic particles. In panel (a) we show a planar magnetic particle with $D_{4h}$ symmetry. The currents under the $A_{2g}$ magnetic mode are shown. Panel (b) shows a 3D isotropic magnetic particle with $O_h$ symmetry. The electric response of this particles is also isotropic, but importantly does not occur at the same frequency as the magnetic resonance.

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*Electronic address: willie@lanl.gov*

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