On the Application of Modal Analysis and Group Theory to Understand the Optical Response of a Nanoantenna

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Abstract: Symmetry holds a prominent position in defining the optical response of a nanoantenna. In this work, we harness a mathematical tool, group representation theory, combine it with the eigenmode analysis for a nanoantenna, and illustrate how the symmetry allows or forbids the energetic coupling (i.e., interference) between a nanoantenna's eigenmodes. We do this especially using a nanobar structure and a symmetric cross structure. Further, the consequence of symmetry-breaking is illustrated by an asymmetric cross-shaped nanostructure, i.e., a strong asymmetric Fano-type resonance line shape due to mode interference is observed with the physics behind elaborated. Both numerical and experimental evidences are provided.

Keywords: Eigenmodes, group theory, mode interference and Fano resonance, nanoantennas, symmetry/symmetry breaking, volumetric integral equation (VIE).

Victor Moshchalkov was born in Russia. He received the M.Sc., Ph.D., and “Habilitation” degrees in physics from the Lomonosov Moscow State University, Moscow, Russia, in 1975, 1978, and 1985, respectively. From 1978 to 1988, he was a Research Physicist, Assistant Professor, and Professor with the Lomonosov Moscow State University, Moscow, Russia, where, in 1988, he became Head of the Laboratory of High Temperature Superconductivity. Since 1986, he has held a number of positions as Guest Scientist or Guest Professor with Toronto University, Toronto, ON, Canada, TH Darmstadt, Marburg University, Marburg, Germany, RWTH Aachen, Aachen, Germany, Centre d’Etudes Nucléaires de Grenoble, Grenoble, France. In 1991, he joined the Katholieke Universiteit Leuven, Leuven, Belgium, as a Visiting Professor, where he became a Full Professor in 1993. He has over 780 publications in international peer reviewed journals and more than 9300 citations. Prof. Moshchalkov is an American Physical Society Fellow since 2007. He was the Chairman of the ESF Program “Vortex Matter in Superconductors VORTEX” from 1999 until 2004. He became the Director of the INPAC Institute for Nanoscale Physics and Chemistry (Center of Excellence at the KU Leuven) in 2005. Since 2007, he is also the Chairman of the ESF-NES program, which includes 60 teams.
from 15 European countries. He was an invited speaker at 96 international conferences and workshops, and he is Founder of the new series of International Conferences on “Vortex Matter in Nanostructured Superconductors.” He is a member of the International Advisory Committee of 34 international conferences. He has been, or is, Promoter of 57 Ph.D. theses (12 at the Moscow State University and 45 at the K.U. Leuven). He was the recipient of several awards: the Young Researcher award in 1986, the High Education Scientific Prize in 1988, the ISI Thomson Scientific Award “Top Cited Paper in Flanders” in 2000, the Dr. A.De Leeuw-Damry-Bourlart Prize for Exact Sciences from the Flemish FWO in 2005, and the Methusalem Research Award in 2009. He was a finalist for the EU Descartes Research Prize in 2006.

Guy A. E. Vandenbosch (F’13) received the M.S. and Ph.D. degrees in electrical engineering from the Katholieke Universiteit Leuven, Leuven, Belgium, in 1985 and 1991, respectively. Since 1993, he has been a Lecturer, and since 2005, a Full Professor at the same university. He has taught or teaches courses on “electromagnetic waves,” “antennas,” “electromagnetic compatibility,” “electrical engineering, electronics, and electrical energy,” and “digital steer-and measuring techniques in physics.” His research interests include the area of electromagnetic theory, computational electromagnetics, planar antennas and circuits, nano-electromagnetics, EM radiation, EMC, and bio-electromagnetics. His has authored 210 papers in international journals and has ca. 300 presentations at international conferences. From 2001 to 2007, he was the President of SITEL, the Belgian Society of Engineers in Telecommunication and Electronics. From 2008–2014, he was a member of the board of FITCE Belgium, the Belgian branch of the Federation of Telecommunications Engineers of the European Union. In 1999–2004, he was vice-chairman, and in 2005–2009 secretary of the IEEE Benelux Chapter on Antennas en Propagation. Currently, he holds the position of chairman of this Chapter. In 2002–2004, he was the secretary of the IEEE Benelux Chapter on EMC. He is currently the secretary of the Belgian National Committee for Radio-electricity (URSI), where he is also in charge of commission E.

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Outline

– Introduction: Interaction between Light and Nanoantennas
– Standard Eigenvalue Problem
– Orthogonality of Eigenmodes and Group Representation Theory
– Conclusions
Introduction
The effect of miniaturization

1. Working frequencies (Optical) - Metals – Reduced Conductivity

- Skin depth ~ Thickness of nanoantennas

- Surface Current -> Volumetric Current

2. Metals - Dispersion
Numerical methods in the analysis of nanoantennas

An **more effective and economical** way to test and validate our ideas:

<table>
<thead>
<tr>
<th>Method</th>
<th>Time domain</th>
<th>Frequency Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Differential Equation Based Method</td>
<td>FDTD</td>
<td>FEM</td>
</tr>
<tr>
<td>(Discretize entire space)</td>
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<td></td>
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<tr>
<td>Integral Equation Based Method</td>
<td>T-MoM</td>
<td>VIE - V-MoM</td>
</tr>
<tr>
<td>(Discretize the volume where the current is flowing)</td>
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</tbody>
</table>
Local Response Theory: The interaction of light with a nanoantenna

A General Relation:

\[ E_{\text{tot}} (r) = E_{\text{inc}} (r) + E_{\text{scat}} (r) \quad r \in \text{Space} \]

At the nanoantenna:

\[ E_{\text{tot}} (r) = \frac{J_{\text{ind}} (r)}{j \omega (\varepsilon (r, \omega) - \varepsilon_0)} \quad \text{Local Response} \]

\[ E_{\text{scat}} (r, \omega) = -j \omega \mu_0 \int_V \overline{G}(r, r', \omega) \cdot J_{\text{ind}} (r', \omega) dv'. \]

The Induced Current:

\[ Z (J_{\text{ind}} (r)) = E_{\text{inc}} (r) \quad r \in V \]

\[ J_{\text{ind}} (r) = Z^{-1} (E_{\text{inc}} (r)) \quad r \in V \]
Numerical Solution – V-MoM

\[ Z \left( \sum_{\text{ind}} d(f_i)(r) \right) E_{\text{inc}} E(r)(r) \in r \in V \]

Testing Procedure:
\[ \langle f_j, Z \left( \sum c_i f_i \right) \rangle = \langle f_j, E_{\text{inc}} \rangle \]

Matrix Form:
\[ \{ z_{ij}(\omega) \} \{ c_i \} = \{ e_j \} \]

Current Solved:
\[ J_{\text{ind}}(r) = \sum c_i f_i(r) r \in V \]

Field at all space points:
\[ E_{\text{scat}}(r) = L \left( J_{\text{ind}}(r') \right) r' \in V, r \in V \]
An Example: Dimer

W = 135 nm, L = 100nm, H = 50 nm, Gap = 20nm

Real Frequency (THz)
Problem solved?

Good News: We can in principle predict the EM fields at all space points for a *given* incident field.

Bad News: Incident Field Dependent …

Q: *Independent* from the excitation?
Standard eigenvalue problem for a nanoantenna

\[ Z \left| J_{\text{ind}}(\mathbf{r}) \right\rangle = E_{\text{inc}}(\mathbf{r}) \]

Eigenvalue problem for a nanoantenna \[^{[1]}\]:

\[ Z \left| J_{i}(\mathbf{r}, \omega) \right\rangle = \lambda_{i}(\omega) \left| J_{i}(\mathbf{r}, \omega) \right\rangle \]

L1 – L4 are extracted at 600 THz

\[ [1] \text{ C. E. Baum, “Emerging technology for transient and broad-band analysis and synthesis of antennas and scatterers,” Proc. IEEE, 64, 1598-1616.} \]
Properties of eigenvalues: Response (I)

Response to a given incident light: \[ Z \left| J(r, \omega) \right\rangle = E_{\text{inc}}(r, \omega) \]

Eigenmode expansion of currents\(^{[1]}\): \[ J(r, \omega) = \sum_{i} c_i J_i(r, \omega) \]

Orthogonality of eigenmodes: \[ \langle J_i(r, \omega), J_j(r, \omega) \rangle = \int_{V'} J_i(r, \omega) \cdot J_j(r, \omega) dv' = \delta_{ij} \]

The coupling coefficients: \[ c_i(\omega) = \frac{\langle J_i(r, \omega), E_{\text{inc}}(r, \omega) \rangle}{\lambda_i(\omega)} \]

Minimum = Resonance
Properties of eigenvalues: Response (II)

W = 70 nm, L = 370 nm, H = 50 nm
Disentangle the material and the geometry

\[ Z \left| J_i (r, \omega) \right\rangle = \lambda_i (\omega) \left| J_i (r, \omega) \right\rangle \]

\[(Z_{tot} + Z_{scat}) \left| J_i (r, \omega) \right\rangle = \lambda_i (\omega) \left| J_i (r, \omega) \right\rangle \]

\[ Z_{tot} \left| J_i (r, \omega) \right\rangle = \frac{1}{j \omega (\varepsilon(\omega) - \varepsilon_0)} J_i (r, \omega) \]

\[ Z_{scat} \left| J_i (r, \omega) \right\rangle = j \omega \mu_0 \int_{V'} \mathbf{G}(r, r', \omega) \cdot \mathbf{J}_i (r', \omega) dV' \]

1. The eigenmode is \textit{completely} defined by the geometry.

\[ Z_{scat} \left| J_i (r, \omega) \right\rangle = \lambda_{scat, i} (\omega) \left| J_i (r, \omega) \right\rangle \]

2. The response is the result of both the geometry and the plasmonic material.

\textbf{Eigenvalue:} \hspace{1cm} \lambda_i (\omega) = \lambda_{mat} (\omega) + \lambda_{scat, i} (\omega)
Properties of eigenmodes: Orthogonality

Orthogonal in a “reaction” sense [1-3]

$$\langle J_i(r, \omega), J_j(r, \omega) \rangle = \int_{V'} J_i(r, \omega) \cdot J_j(r, \omega) dV' = \delta_{ij}$$

NOT Orthogonal in a “power” sense

$$\langle J_i^*(r, \omega), J_j(r, \omega) \rangle = \int_{V'} J_i^*(r, \omega) \cdot J_j(r, \omega) dV' = \delta_{ij}$$


Properties of eigenmodes: Interference

When evaluating the power delivered from incident light to a nanoantenna:

\[ P = \langle J^* (\mathbf{r}, \omega), E_{\text{inc}} (\mathbf{r}, \omega) \rangle \]

\[ = \sum_{ij} c_j c_i \lambda_i (\omega) \langle J_j^* (\mathbf{r}, \omega), J_i (\mathbf{r}, \omega) \rangle \]

\[ = \sum_{ij} c_j c_i z_{ji} (\omega) \]

Cross Term = Interference

\[ J(\mathbf{r}, \omega) = \sum_i c_i J_i (\mathbf{r}, \omega) \]

\[ E_{\text{inc}} (\mathbf{r}, \omega) = Z |J(\mathbf{r}, \omega)| = \sum_i c_i \lambda_i (\omega) J_i (\mathbf{r}, \omega) \]

Mutual Impedance

Properties of eigenmodes: Spectral Features

Properties of eigenmodes: Interference

... the mirroring symmetry divides the modes into two orthonormal sets ...
Properties of eigenmodes: Group Theory

Two functions which belong to different irreducible representations or to different rows (if the representation is in matrix form) of the same unitary representation are orthogonal in an inner product sense.” [1-2]

Properties of eigenmodes: Symmetric Cross Structure (I)

\[ G = \{E, A, B, C, D, F, G, H\} \]

<table>
<thead>
<tr>
<th>( \Gamma_1 )</th>
<th>( \Gamma_2 )</th>
<th>( \Gamma_3 )</th>
<th>( \Gamma_4 )</th>
<th>( \Gamma_5 )</th>
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<tr>
<td>B</td>
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</tr>
<tr>
<td>A</td>
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<td>1</td>
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<tr>
<td>B</td>
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<tr>
<td>C</td>
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<tr>
<td>D</td>
<td>1</td>
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<tr>
<td>F</td>
<td>1</td>
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<tr>
<td>G</td>
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</tr>
<tr>
<td>H</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
Properties of eigenmodes: Symmetric Cross Structure (II)
Properties of eigenmodes: Asymmetric Cross Structure (I)

\[ D_4 : G = \{ E, A, B, C, D, F, G, H \} \]

\[ C_2 : G = \{ E, m_v \} \]

\[
\begin{array}{cccccccc}
E & A & B & C & D & F & G & H \\
\Gamma_1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\Gamma_2 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\
\Gamma_3 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\
\Gamma_4 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\
\Gamma_5 & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \\
\end{array}
\]
Properties of eigenmodes: Asymmetric Cross Structure (II)
Properties of eigenmodes: Asymmetric Cross Structure (III)
Properties of eigenmodes: Chiral Structure (I)

$C_4$ Group (Abelian)

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$C_4^1$</th>
<th>$C_4^2$</th>
<th>$C_4^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td>$\Gamma_2$</td>
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<td>-1</td>
</tr>
<tr>
<td>$\Gamma_3$</td>
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<td>i</td>
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<td>-i</td>
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<tr>
<td>$\Gamma_4$</td>
<td>1</td>
<td>-i</td>
<td>-1</td>
<td>i</td>
</tr>
</tbody>
</table>
Properties of eigenmodes: Chiral Structure (II)
Conclusions

- Volume Integral Equation: Interaction between Light and Nanoantennas
- Standard Eigenvalue Problem
- Eigenmodes Orthogonality and Group Representation Theory