Bianisotropy and Chirality

Neal, Palffy-Muhoray

- for negative index, need $\varepsilon < 0, \quad \mu < 0$
- conventional idea:

$$\mathbf{D} = \varepsilon \mathbf{E}$$
$$\mathbf{H} = \mu^{-1} \mathbf{B}$$

  - use wires — for negative epsilon
  - use resonators — for negative mu
- bianisotropic media:

$$\mathbf{D} = \varepsilon \mathbf{E} + \alpha \mathbf{B}$$
$$\mathbf{H} = \beta \mathbf{E} + \mu^{-1} \mathbf{B}$$

- idea of NIM via chirality:
  - use β and $\mathbf{E}$-field to produce $\mathbf{H}$ out of phase with $\mathbf{B}$

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NIMs MURI

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1

The bianisotropic formalism has been proposed without firm justification.

It works reasonably well for optically active materials, with relatively small optical activity.

The basis of optical activity is non-locality; the dipole moment depends not only on the field, but also the gradients of the field.

Alternative descriptions (Landau, Agranovich) with k-dependent susceptibilities are better justified, and likely give better description of systems which are strongly non-local.

Negative mu means that H and B are out of phase.

In principle, if BA formalism is correct, and beta is sufficiently large, H may be out of phase with B due to the contribution of E.

Question: does the BA formalism work for NPs in NIMs?

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- Question:
  - does BA formalism describe well the response of metallic NPs in NIMs at optical frequencies?
- BA formalism implies that for constituent particles

$$\mathbf{p} = \overline{\overline{\alpha}}\mathbf{E} + \overline{\overline{\beta}}\mathbf{B}$$
$$\mathbf{m} = \overline{\overline{\gamma}}\mathbf{E} + \overline{\overline{\delta}}\mathbf{B} \qquad (3)$$

  where the susceptibilities are independent of the wave vector

- numerical simulations for pairs of Au NW using the *discrete dipole approximation* to check the validity of these equations

The BA formalism predicts that the particle susceptibilities depend on both B and E fields, as given above.

DDA simulation details

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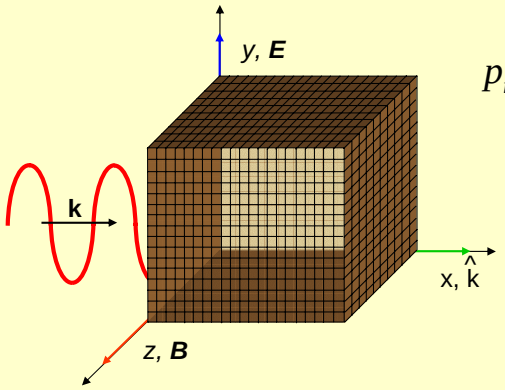
- Discrete dipole approximation (DDA) simulation determines susceptibilites



Simulation Solves:

$$p_i = \alpha_i (E_{inc,i} - \sum_{j \neq k}^{N} A_{jk} p_k)$$

If

$$\alpha_i^{-1} = A_{ii}$$

then

$$\sum_{i=1}^{N} A_{ij} p_i = E_{inc,j}$$

DDA is an accurate method to determine the material response

This can be used to check validity of BA formalism

We can determine the dipole moments using this scheme, and see if they have the field dependence predicted by the BA formalism.

Results: computed dipole moments for Au NRs

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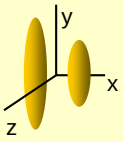

1 P_{re}=-22839 P_{Im}=19649	2 P_{re}=-25800 P_{Im}=-8808	3 P_{re}=-25046 P_{Im}=4570
4 P_{re}=-25060 P_{Im}=4559	5 P_{re}=7232 P_{Im}=-420	6 P_{re}=7230 P_{Im}=-418
7 P_{re}=6541 P_{Im}=-419	8 P_{re}=6536 P_{Im}=-409	9 P_{re}=6554 P_{Im}=253
10 P_{re}=6513 P_{Im}=-553	11 P_{re}=7382 P_{Im}=163	12 P_{re}=7381 P_{Im}=163

P-complex dipole moment (along y-axis) B-field E-field Wave vector

Calculated electric susceptibilities for pair of Au NRs from DDA computation

Comparison of BA predictions and simulations

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	BA Relation	Simulation	
$p_1+p_2-p_3-p_4=$	0	8 %	←
$p_5+p_6-p_{11}-p_{12}=$	0	16 %	←
$p_7+p_8-p_9-p_{10}=$	0	8 %	←
$p_1-p_2-p_5+p_6=$	0	159 %	←
$p_3-p_4-p_7+p_8=$	0	1 %	
$p_9-p_{10}-p_{11}+p_{12}=$	0	11 %	←

Large discrepancies!

If predictions of BA formalism were correct, the dipole sums on left would all be zero.

Simulations give numbers which very significantly differ from zero.

BA does not work well!

Predictions based on BA formalism cannot be relied on to predict response.

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- numerical simulations show that the predictions of BA formalism are not well obeyed .
- BA constitutive relations therefore do not, in general, provide a good description of spatially non-local systems.
- predictions about chiral NIMs based on BA relations may therefore be questionable;
- need better description of non-local response.

Since BA formalism does not appear to work well, its prediction of getting NIM through very strong chirality (large beta) may not hold.