GEneralized Normal Modes Expansion (GENOME) of Green's tensor for open/lossy systems

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Nanolight, Spain, 3/2018

Electrodynamics Simulations

Maxwell's Equations

$$\nabla \times (\nabla \times \boldsymbol{E}(\boldsymbol{r})) - \epsilon(\boldsymbol{r})k^2\boldsymbol{E}(\boldsymbol{r}) = i\omega\mu_0\boldsymbol{J}_f(\boldsymbol{r})$$

- general sources, general structure

Green's Tensor

$$\nabla \times (\nabla \times \overleftrightarrow{G}(\boldsymbol{r},\boldsymbol{r}')) - \epsilon(\boldsymbol{r})k^2\overleftrightarrow{G}(\boldsymbol{r},\boldsymbol{r}') = k^2\overleftrightarrow{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$

- for a point source
- e.g. spontaneous emission rate, (L)DOS, thermal emission, dipole-dipole intn's, …

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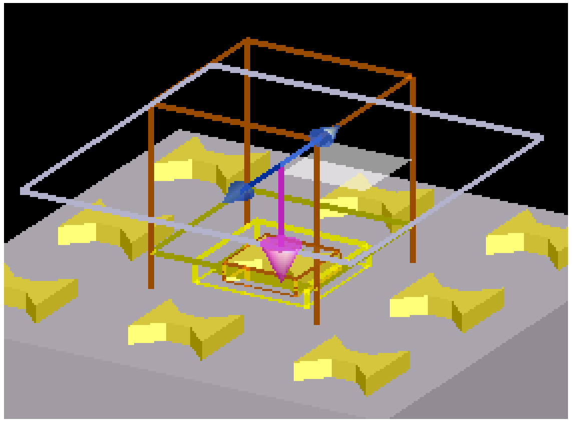

Lumerical FDTD

FDTD/FEM solution

- Define structure & sources
- Repeat simulation for each source distribution
- Hinders study of problems requiring heavy computations

Electrodynamics Simulations – alternative

- eigenmode expansion
  - obtain modes in a single simulation
  - expand fields/Green function in terms of modes

- textbook formulation –

$$\overleftrightarrow{G}(\boldsymbol{r},\boldsymbol{r}') = \sum_m \frac{\boldsymbol{E}_m(\boldsymbol{r})\boldsymbol{E}^*_m(\boldsymbol{r}')}{\lambda_m - \lambda}$$

e.g., Morse & Feshbach 1953

  - E_m called normal modes (stationary solutions)
  - E computed via a superposition integral

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  - open problem!
- in this talk – resolve the problem!

Eigenmode methods – complex frequency (ω) eigenvalues

- Previous derivations of a spectral formulation relied on frequency eigenvalues
  - real part – rate of phase accumulation
  - imaginary part – mode lifetime
- Called quasi-normal modes

- Lalanne group, Hughes group, Muljarov group, Kuipers group, …

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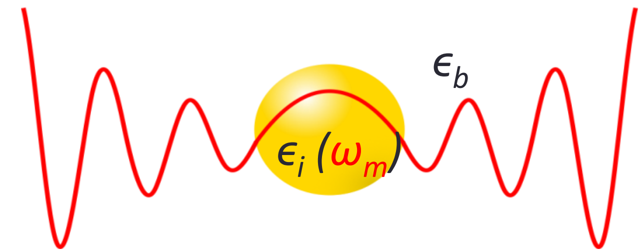
- Example – a single sphere
- Internal field $E \sim (2\epsilon_b + \epsilon_i)^{-1}$
  - (complex) eigen-frequency defines a resonance
  - associated with a long series of complications
    - accepts only analytical models for ϵ
    - modes diverges at infinity
    - non-linear eigenvalue equation
    - approximate: incomplete basis



$$\epsilon_i(\omega_m) = -2\epsilon_b$$

$$\frac{1}{\epsilon(\boldsymbol{r},\omega_m)}\nabla\times(\nabla\times\boldsymbol{E}_m) = \left(\frac{\omega_m}{c}\right)^2\boldsymbol{E}_m$$

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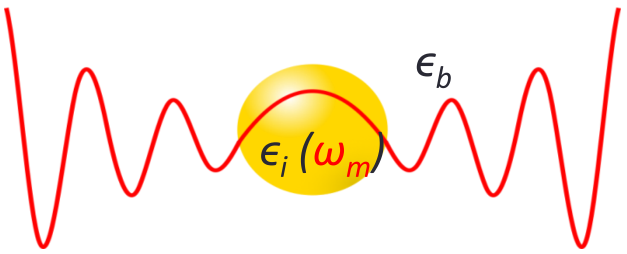

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Eigenmode methods – complex frequency (ω) eigenvalues

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  - real part – rate of phase accumulation
  - imaginary part – mode lifetime
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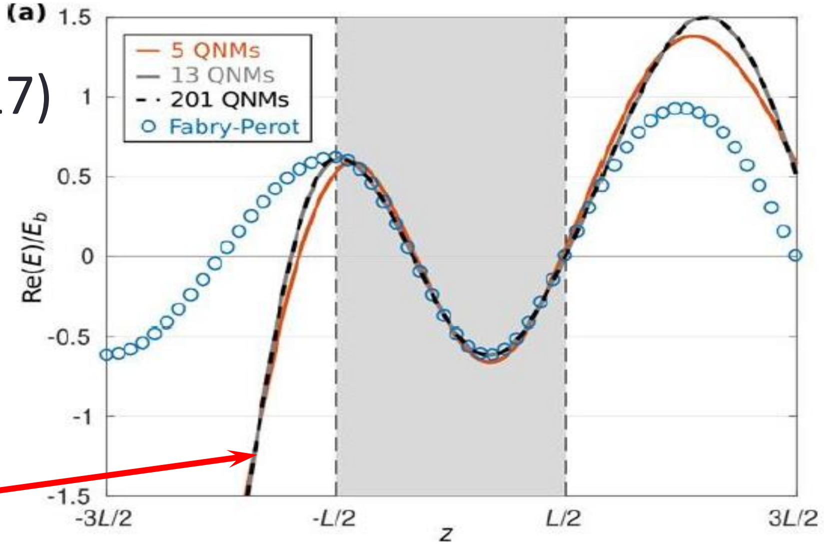
  - Example – 1D slab (Lalanne *et al.*, 2017)
  - Excellent agreement inside the slab
  - Fields outside slab totally wrong; increasing # of modes does not help



Eigenmode methods – complex permittivity (ϵ) eigenvalues

- Previous derivations of a spectral formulation relied on frequency eigenvalues
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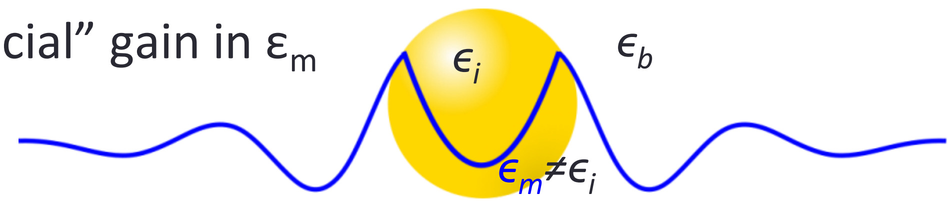
  - imaginary part – mode lifetime

- Alternative – permittivity (ϵ) eigenvalues
  - radiation loss compensated by "artificial" gain in ε_m
  - decay in space
- Normal modes!



$$\epsilon_m = -2\epsilon_b$$

- Previous work – Bergman (1979 –), Agranovitch group, Stone group (SALT)

Eigenmode methods – complex permittivity (ϵ) eigenvalues

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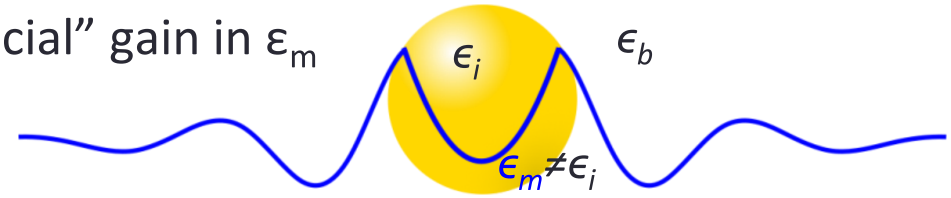
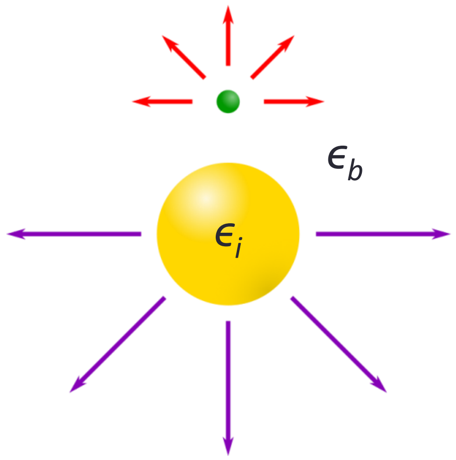
- In this talk
  1. simple derivation
  2. expression for Green's tensor
  3. easy numerical implementation



$$\epsilon_m = -2\epsilon_b$$

Derivation I



Begin with Helmholtz equation with sources

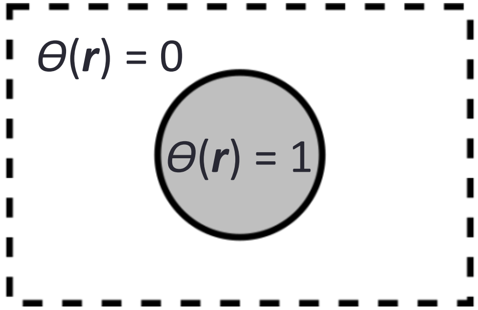
$$\nabla \times (\nabla \times \boldsymbol{E}(\boldsymbol{r})) - \epsilon(\boldsymbol{r})k^2\boldsymbol{E}(\boldsymbol{r}) = i\omega\mu_0\boldsymbol{J}_f(\boldsymbol{r})$$

Treat structure as another source of inhomogeneity

$$\nabla \times (\nabla \times \boldsymbol{E}) - \epsilon_b k^2\boldsymbol{E} = (\epsilon_i - \epsilon_b)\theta(\boldsymbol{r})k^2\boldsymbol{E} + i\omega\mu_0\boldsymbol{J}_f(\boldsymbol{r})$$

by moving to Right-Hand-Side

$\Theta(\boldsymbol{r})$ = Heaviside function



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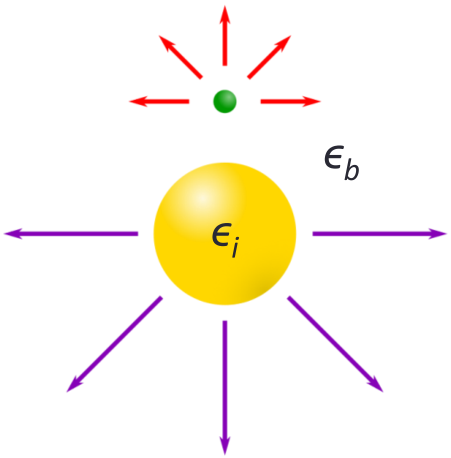

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Green's function solution (Lippmann-Schwinger)

$$\boldsymbol{E}(\boldsymbol{r}) = \underbrace{(\epsilon_i - \epsilon_b)}_{u} \underbrace{\int \overleftrightarrow{G}_0(|\boldsymbol{r} - \boldsymbol{r}'|)}_{\hat{\Gamma}} \underbrace{\theta(\boldsymbol{r}')}_{\hat{\theta}} \boldsymbol{E}(\boldsymbol{r}')\, d\boldsymbol{r}' + \frac{i}{\omega\epsilon_0} \underbrace{\int \overleftrightarrow{G}_0(|\boldsymbol{r} - \boldsymbol{r}'|)}_{\hat{\Gamma}} \boldsymbol{J}_f(\boldsymbol{r}')\, d\boldsymbol{r}'$$

where $\nabla \times (\nabla \times \overleftrightarrow{G}_0) - \epsilon_b k^2 \overleftrightarrow{G}_0 = k^2 \overleftrightarrow{\delta}(\boldsymbol{r} - \boldsymbol{r}')$

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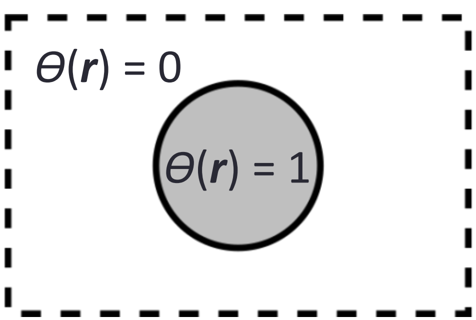

In absence of a source, get an eigenvalue problem

$$\boldsymbol{E}_m(\boldsymbol{r}) = \underbrace{(\epsilon_m - \epsilon_b)}_{u_m} \underbrace{\int \overleftrightarrow{G}_0(|\boldsymbol{r} - \boldsymbol{r}'|)}_{\hat{\Gamma}} \underbrace{\theta(\boldsymbol{r}')}_{\hat{\theta}} \boldsymbol{E}_m(\boldsymbol{r}') d\boldsymbol{r}' \Longrightarrow \langle E_m | \hat{\Gamma}\hat{\theta} = \frac{1}{u_m} \langle E_m |$$

Derivation II

$$\boldsymbol{E}(\boldsymbol{r}) = \underbrace{(\epsilon_i - \epsilon_b)}_{u} \underbrace{\int \overleftrightarrow{G}_0(|\boldsymbol{r}-\boldsymbol{r}'|)}_{\hat{\Gamma}} \underbrace{\theta(\boldsymbol{r}')}_{\hat{\theta}} \boldsymbol{E}(\boldsymbol{r}')\, d\boldsymbol{r}' + \frac{i}{\omega\epsilon_0} \underbrace{\int \overleftrightarrow{G}_0(|\boldsymbol{r}-\boldsymbol{r}'|)}_{\hat{\Gamma}} \boldsymbol{J}_f(\boldsymbol{r}')\, d\boldsymbol{r}'$$

⟹ Compact notation: $\boldsymbol{E} = u\hat{\Gamma}\hat{\theta}\boldsymbol{E} + \frac{i}{\omega\epsilon_0}\hat{\Gamma}\boldsymbol{J}_f$ Farhi & Bergman, *PRA* (2016)

Formal solution: $\boldsymbol{E} = \left(\frac{1}{1 - u\hat{\Gamma}\hat{\theta}}\right) \frac{i}{\omega\epsilon_0}\hat{\Gamma}\boldsymbol{J}_f$

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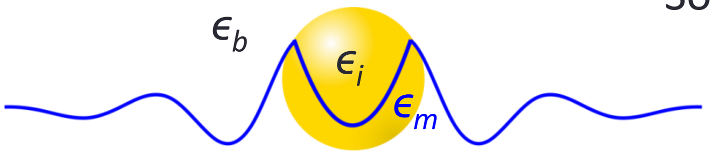


NB: $\epsilon_m \neq \epsilon_i$

Solve by projecting onto eigenmodes (left multiplication)

$$\hat{I} = \sum_m \hat{\theta}|E_m\rangle\langle E_m|\hat{\theta} \qquad \langle E_m|\hat{\Gamma}\hat{\theta} = \frac{1}{u_m}\langle E_m|$$

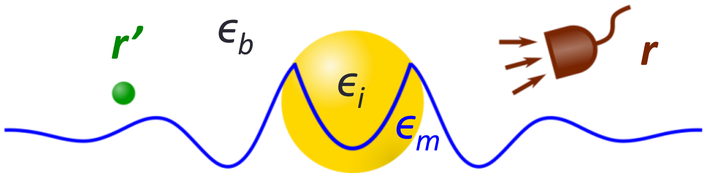
operate to the left (on bra)

$$-i\omega\epsilon_0\hat{\theta}|E\rangle = \sum_m \hat{\theta}|E_m\rangle\langle E_m|\frac{\hat{\Gamma}\hat{\theta}}{1-u\hat{\Gamma}\hat{\theta}}|J_f\rangle = \sum_m \hat{\theta}|E_m\rangle\frac{1}{u_m - u}\langle E_m|J_f\rangle$$

Substituting into the Lippmann-Schwinger equation gives field <u>everywhere</u>

$$-i\omega\epsilon_0|E\rangle = \hat{\Gamma}|J_f\rangle + \sum_m |E_m\rangle\frac{\epsilon_i - \epsilon_b}{(\epsilon_m - \epsilon_i)(\epsilon_m - \epsilon_b)}\langle E_m|J_f\rangle$$

Analytic solution for Fields



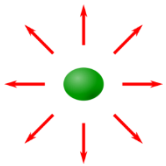
NB: $\epsilon_m \neq \epsilon_i$

Eigenmodes provide total field
for all ***source*** and ***detector*** configurations ***in a single simulation!***

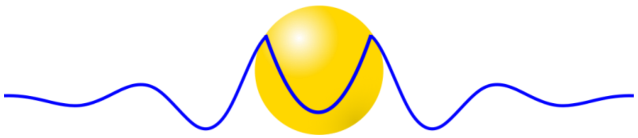
$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}_0(\boldsymbol{r}) + \frac{1}{i\omega\epsilon_0}\sum_m \boldsymbol{E}_m(\boldsymbol{r})\,\frac{\epsilon_i - \epsilon_b}{(\epsilon_m - \epsilon_i)(\epsilon_m - \epsilon_b)}\int \boldsymbol{E}_m^{\dagger}(\boldsymbol{r}')\cdot \boldsymbol{J}_f(\boldsymbol{r}')\,dV$$

radiation
w/o structure

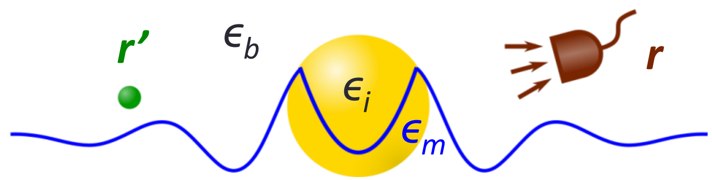
structure w/o radiation



$$\int \overleftrightarrow{G}_0(|\boldsymbol{r}-\boldsymbol{r}'|)\boldsymbol{J}_f(\boldsymbol{r}')\,d\boldsymbol{r}'$$



Analytic solution for Fields



NB: $\epsilon_m \neq \epsilon_i$

Eigenmodes provide total field
for all ***source*** and ***detector*** configurations ***in a single simulation!***

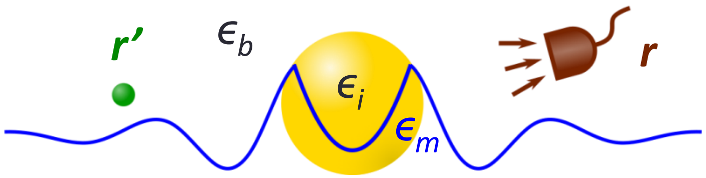
$$\mathbf{E}(\mathbf{r}) = \underbrace{\mathbf{E}_0(\mathbf{r})}_{\text{radiation w/o structure}} + \frac{1}{i\omega\epsilon_0} \sum_m \mathbf{E}_m(\mathbf{r}) \underbrace{\frac{\epsilon_i - \epsilon_b}{(\epsilon_m - \epsilon_i)(\epsilon_m - \epsilon_b)}}_{\text{detuning from resonance}} \underbrace{\int \mathbf{E}_m^{\dagger}(\mathbf{r}') \cdot \mathbf{J}_f(\mathbf{r}')\, dV}_{\text{source-mode overlap}}$$

- Straightforward physical interpretation
- Rigorous everywhere (completeness)
- Applicable to any (complex) inclusion material
- Same analytical form for all sources – far field, near field, …

Analytic solution for Green's Function – I

for a point source:

$$J_f(\mathbf{r}') = J_0\delta(\mathbf{r}')$$



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Eigenmodes provide Green's tensor
for all ***source*** and ***detector*** configurations ***in a single simulation!***

$$\overset{\leftrightarrow}{G}(\mathbf{r},\mathbf{r}') = \underbrace{\overset{\leftrightarrow}{G}_0(|\mathbf{r}-\mathbf{r}'|)}_{\text{free-space Green's tensor}} + \frac{1}{k^2}\sum_m \mathbf{E}_m(\mathbf{r}) \underbrace{\frac{\epsilon_i-\epsilon_b}{(\epsilon_m-\epsilon_i)(\epsilon_m-\epsilon_b)}}_{\text{detuning from resonance}} \mathbf{E}_m^\dagger(\mathbf{r}')$$

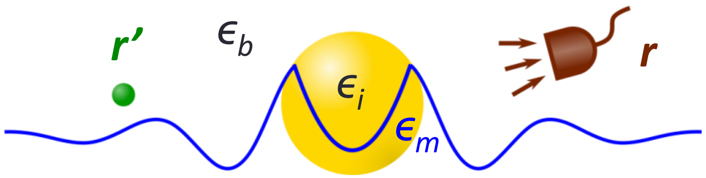
free-space
Green's tensor

detuning
from resonance

Analytic solution for Green's Function – II

for a point source:

$$J_f(\mathbf{r}') = J_0\delta(\mathbf{r}')$$



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- Different from "standard" Green function expansion
  - valid for lossy and/or open systems
  - includes source
  - rigorous everywhere (completeness)
  - extra factor vanishes on resonance

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}') = \sum_m \frac{\mathbf{E}_m(\mathbf{r})\mathbf{E}_m^*(\mathbf{r}')}{\lambda_m-\lambda}$$

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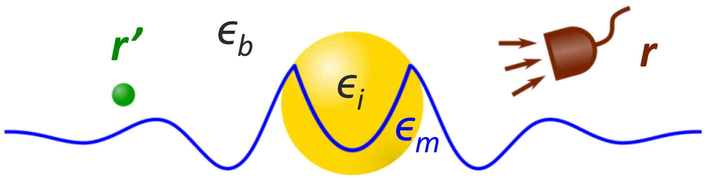

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free-space
Green's tensor

detuning
from resonance

GEneralised Normal Mode Expansion – GENOME

Chen, Bergman & Sivan, ArXiv

Finding the ϵ-Eigenmodes

<u>Analytic</u>

spheres, slabs, cylinders

For simple structures solve dispersion relation

$$n\frac{j_m'(na)}{j_m(na)} = \frac{y_m'(a)}{y_m(a)}$$

$$\left(\frac{\mu_c}{\alpha_c a}\frac{J}{J}\cdots\right)\left(\frac{\epsilon_c}{\alpha_c a}\frac{J_m'(\alpha_c a)}{J_m(\alpha_c a)} - \frac{\epsilon_b}{\alpha_b a}\frac{H_m'(\alpha_b a)}{H_m(\alpha_b a)}\right) - \left(\frac{m\beta}{k}\right)^2\left(\frac{1}{(\alpha_c a)^2} - \frac{1}{(\alpha_b a)^2}\right)^2 = 0$$

e.g., sphere dispersion relation

solve by contour methods (Chen & Sivan, Comp. Phys. Comm. 2017)

Comparison to Mie Solution

Line dipole source near cylinder; G_{xx} component of the electric field

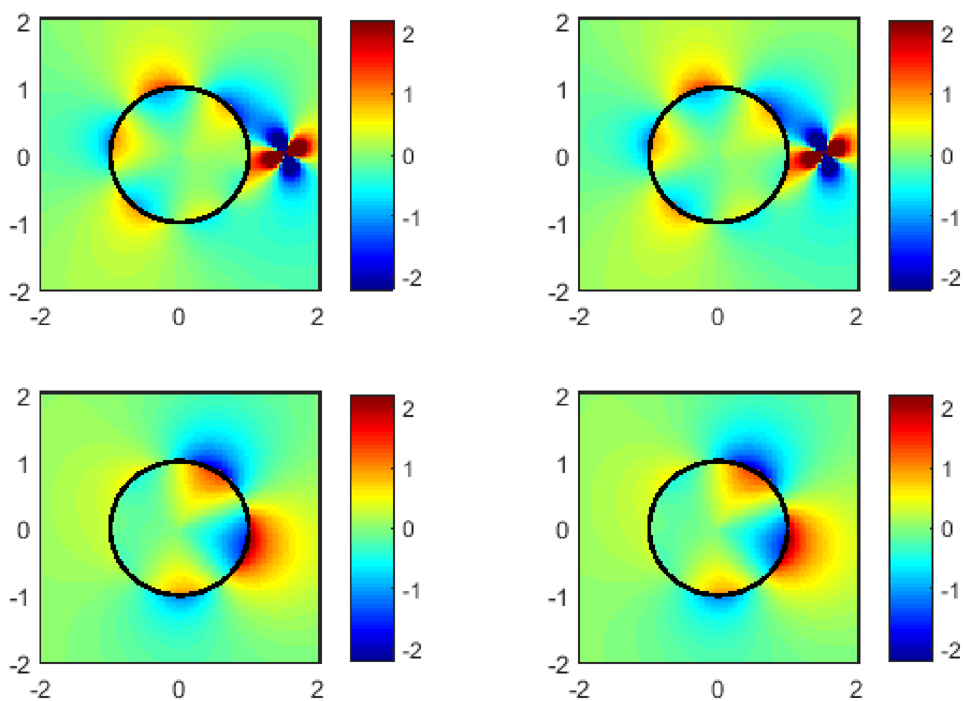
On Resonance

$ka = 1$, $\varepsilon_m = -1.4+0.2i$, $\varepsilon_i = -1.4-0.2i$, source at $1.5a$

Mie GENOME

Real

Imaginary



Eigenmode search: PY Chen, Y Sivan, *CPC* **214** 105 (2017); free codes!

Comparison to Mie Solution

Line dipole source near cylinder; Arbitrary close to Mie solution

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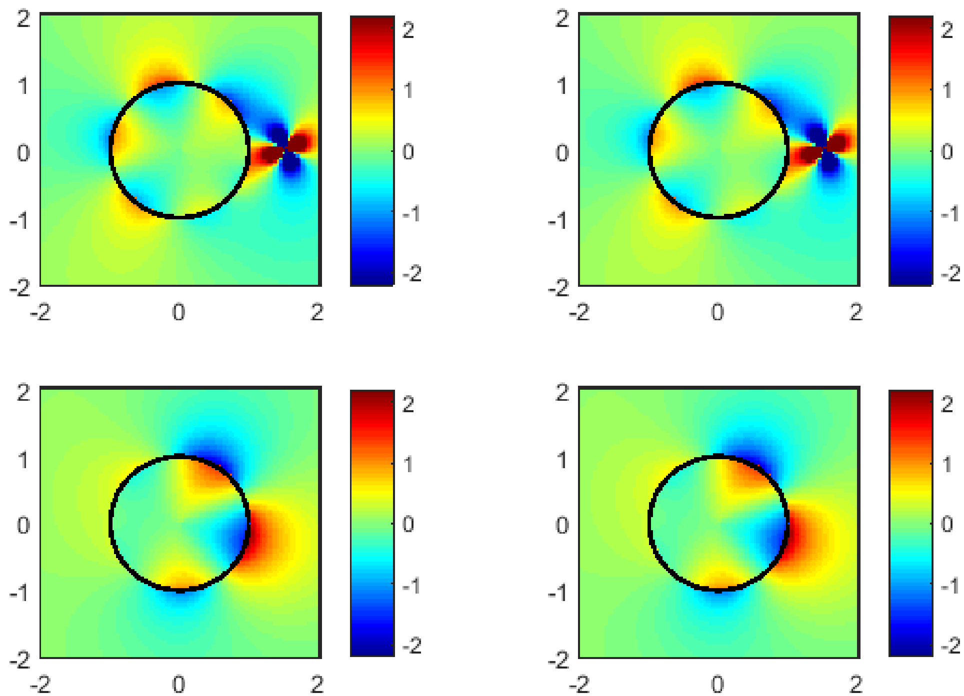
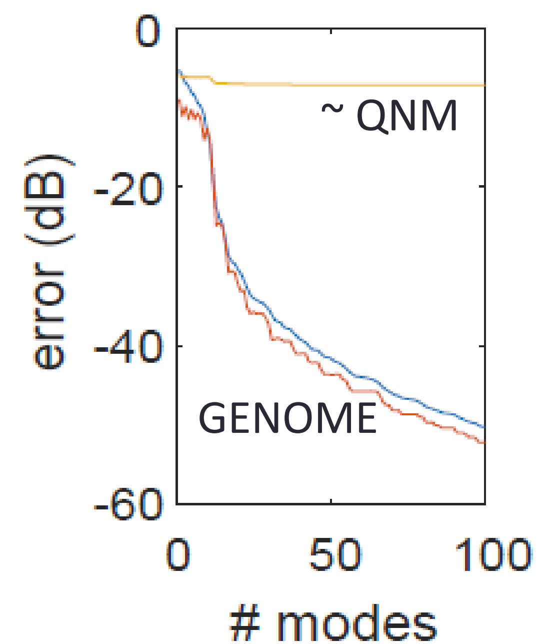




- inside and arbitrarily far outside cylinder
- including source..
- Imaginary and real part

Eigenmode search: PY Chen, Y Sivan, *CPC* **214** 105 (2017); free codes!

Comparison to Mie Solution

Line dipole source near cylinder; Arbitrary close to Mie solution

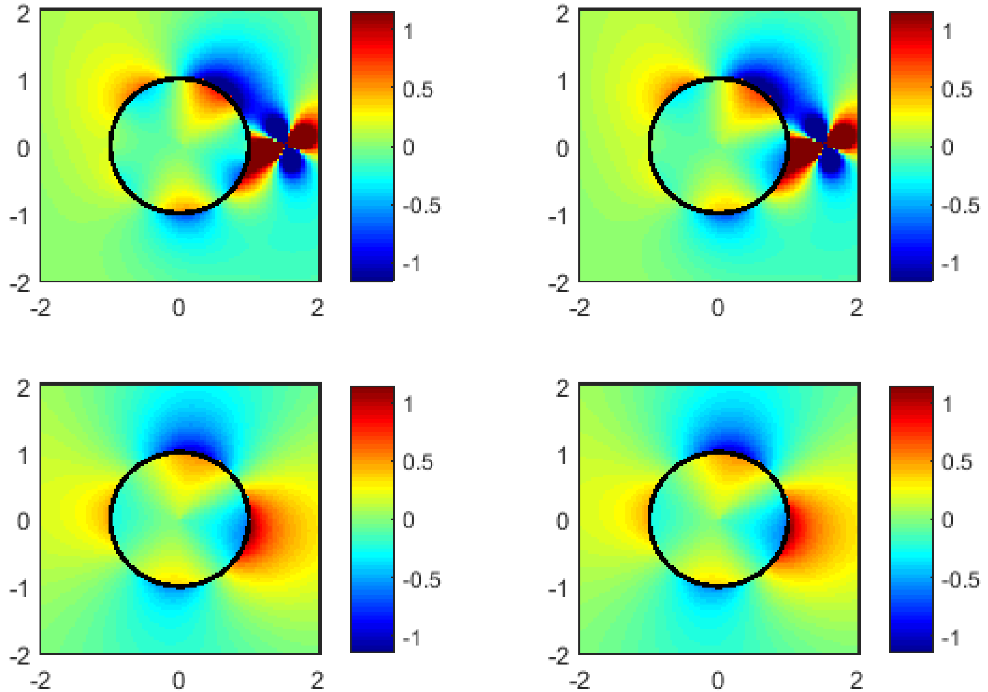
Half Maximum

$ka = 1$, $\varepsilon_m = -1.4+0.2i$, $\varepsilon_i = -2-0.2i$, source at $1.5a$

Mie GENOME

Real

Imaginary



- on and off resonance

Eigenmode search: PY Chen, Y Sivan, *CPC* **214** 105 (2017); free codes!

General structure – COMSOL implementation

Eigenvalue equation – differential form

$$\nabla \times (\nabla \times \boldsymbol{E}_m) - \epsilon_b k_0^2 \boldsymbol{E}_m = (\epsilon_m - \epsilon_b)\theta(\boldsymbol{r}) k_0^2 \boldsymbol{E}_m$$

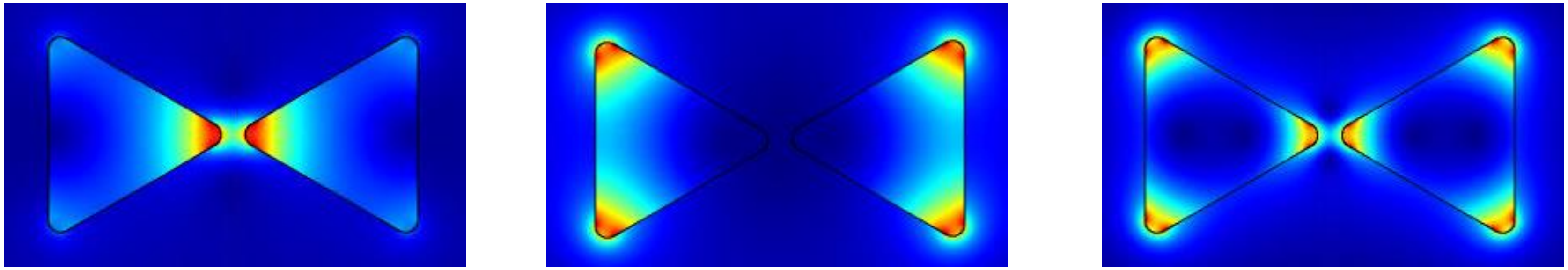
However, COMSOL only solves for *k* as eigenvalue

$$\nabla \times (\nabla \times \boldsymbol{E}_m(\boldsymbol{r})) - \tilde{\epsilon}(\tilde{\omega}, \boldsymbol{r}) \tilde{k}_m^2 \boldsymbol{E}_m(\boldsymbol{r}) = 0$$

solved by simple substitution trick

Results

Bowtie antenna



ϵ_m = 0.28+0.056i ϵ_m = 0.42+0.016i ϵ_m = 0.56+0.009i

Chen, Bergman & Sivan, ArXiv

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Results

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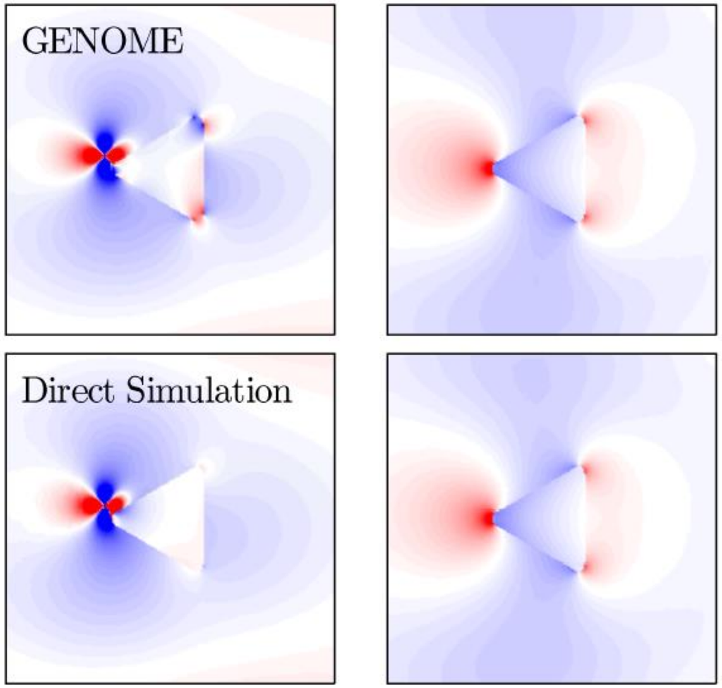
- agreement up to 2-3 digits with < 10 modes

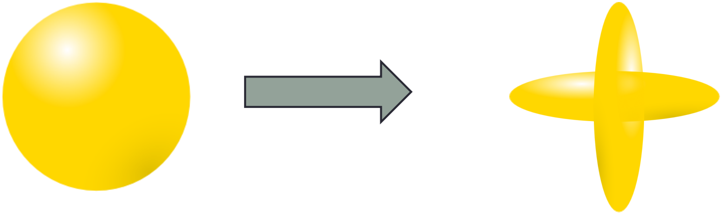


Real(G_{xx}) Imag(G_{xx})

Chen, Bergman & Sivan, ArXiv

Extensions – I

- Compute modes of “distorted” geometries semi-analytically
  - with E. Muljarov, Cardiff
  - reliable eigenvalue solver for any geometry; inhomogeneous permittivity
  - exact solution without solving any PDE!



“distortions” can be *arbitrarily deep due to completeness*

~ 100 times faster than COMSOL; fully reliable

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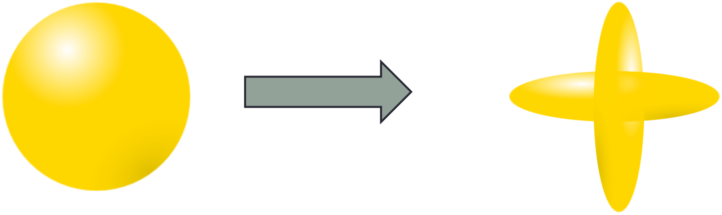

"distortions" can be *arbitrarily deep due to completeness*

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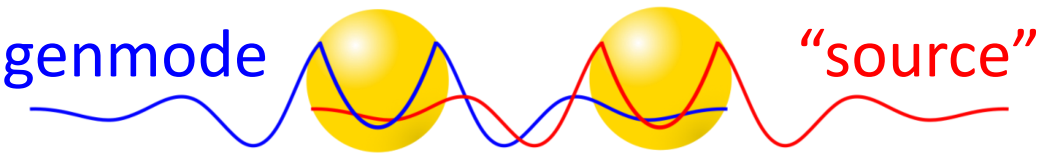
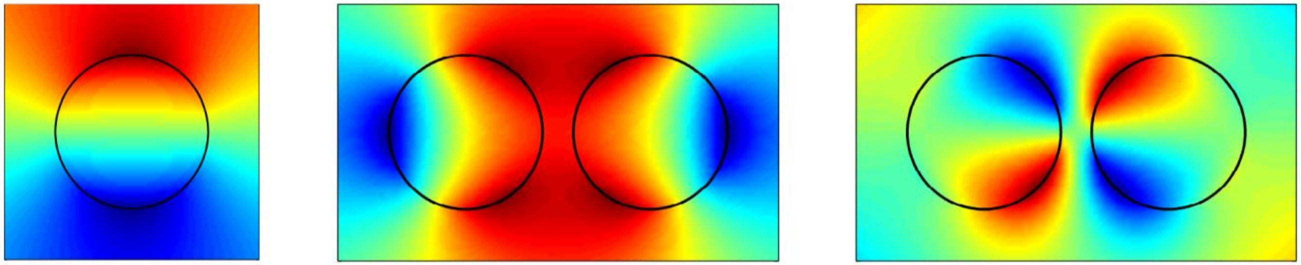
- "Distort" frequency
  - obtain lineshapes from a single calculation
  - overcome only advantage of quasi-normal modes…

Additional results

- Exact version of "hybridization theory"



Two Cylinder Modes



- Extend formulation to periodic systems (underway)
- Solve an old problems in nonlinear optics – surface nonlinearity [Reddy et al. JOSAB (2017)]
- Extend to magnetic materials [Bergman, Farhi, Chen, submitted]

Summary – I

- Generalization of normal mode expansions to lossy/open systems (GENOME)
  - solve problem that was open for decades
- Orders-of-magnitude faster than “brute-force” numerics
- Exact; compatible with any numerical scheme currently in use..
- Deep physical insights
  - modal contribution, interference and competition, …

Summary – II

- Especially useful for computationally-heavy problems
  - Metamaterial design, thermal emission, heat transfer, …
  - Purcell effect calculations
    - e.g., graphene flakes..
  - vdW forces, quantum friction, …
  - Forster energy transfer
  - …
- Looking for interesting problems & interested colleagues…
  - experimentalists , theoreticians, numerics experts, …
  - open positions for students/post docs