Rigorous Quality Factor Calculation in Contemporary Optical Resonant Systems

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**Motivation**

- Resonant structures are ubiquitous in modern photonics integrated circuits
- Contemporary platforms (plasmonics) and materials (graphene) exhibit distinct characteristics
- Quality factor calculation is non-trivial

**Objectives**

- Collectively present the $Q$-factor calculation techniques using commercially available software implementing FEM (COMSOL Multiphysics, ANSYS HFSS, CST Microwave studio)
- Highlight the effect of material dispersion, ohmic loss and light leakage on the calculations
- Propose alternatives routes
Presentation outline

- **Computational methods for calculating the Quality Factor**
  1. Eigenvector
  2. Field distribution
  3. Eigenfrequency
  4. Spectral response

- **Application range of the methods via examples**
  - Silicon ring resonator at the NIR
  - Graphene tube resonator at the FIR
  - Polaritonic rod at the FIR
  - Plasmonic core-shell at the visible

- **Conclusions**
Computational methods for calculating the Quality Factor
Quality factor definition (1): the eigenmode and the field distribution methods

Quality Factor definition

\[ Q = \omega_0 \frac{W}{P_{\text{loss}}} \]

- \( W \) Stored energy on resonance
- \( P_{\text{loss}} \) Power loss

\[ P_{\text{loss}} = \{ P_{\text{res}}, P_{\text{rad}}, P_i, P_e, P_\ell \} \]

- Resistive
- Radiation
- External (coupling)
- Intrinsic
- Loaded

[D. M. Pozar, Microwave Engineering]
Quality factor definition (1): the *eigenmode* and the *field distribution* methods

**Quality Factor definition**

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- Resistive \( \quad \) Intrinsic
- Radiation \( \quad \) Loaded
- External (coupling) \( \quad \)

[D. M. Pozar, Microwave Engineering]

**Energy and Losses calculation**

\[ W = \frac{1}{4} \int_V \varepsilon_0 \frac{\partial \{ \omega \varepsilon_r (\omega) \}}{\partial \omega} |\mathbf{E}|^2 \, d\mathbf{r} + \frac{1}{4} \int_V \mu_0 |\mathbf{H}|^2 \, d\mathbf{r} + \frac{1}{4} \int_V \frac{\partial \mathrm{Im} \{ \sigma (\omega) \}}{\partial \omega} |\mathbf{E}|^2 \, d\mathbf{r} \]

Material dispersion

\[ P_{\text{res}} = \frac{1}{2} \int_V \Re \{ \mathbf{E} \cdot \mathbf{J}^* \} \, d\mathbf{r} = \frac{1}{2} \int_V \Re \{ \sigma \} |\mathbf{E}|^2 \, d\mathbf{r} + \frac{1}{2} \int_V \omega \varepsilon_0 \mathrm{Im} \{ \varepsilon_r \} |\mathbf{E}|^2 \, d\mathbf{r} \]

Ohmic loss

\[ P_{\text{rad}} = \int_{\partial V} \Re \{ \mathbf{S}_c \} \cdot \hat{n} \, d\mathbf{r} = \frac{1}{2} \int_{\partial V} \Re \{ \mathbf{E} \times \mathbf{H}^* \} \cdot \hat{n} \, d\mathbf{r} \]

\[ P_e = \int_{\text{wg}} \Re \{ \mathbf{S}_c \} \cdot \hat{n} \, d\mathbf{r} = \frac{1}{2} \int_{\text{wg}} \Re \{ \mathbf{E} \times \mathbf{H}^* \} \cdot \hat{n} \, d\mathbf{r} \]

\[ \frac{1}{Q_{\ell}} = \frac{1}{Q_i} + \frac{1}{Q_e} = \frac{1}{Q_{\text{res}}} + \frac{1}{Q_{\text{rad}}} + \frac{1}{Q_e} \]
Quality factor definition (2): the eigenmode and the field distribution methods

1. The eigenmode method
   - Complex eigenvalue $\tilde{\omega} = \omega' + j\omega''$
   - Temporal decay $\propto \exp\{-\omega''t\}$
   - Spatial exponential divergence! $\propto \exp\{+r\omega''/c\}$

   ![Diagram showing the field distribution and radial distance](image)

   - $W$ and $P_{loss}$ diverge but $W/P_{loss}$ is constant

   $P_{rad} + P_e = 2\omega''W - P_{res}$

   [L. D. Landau, Electrodynamics of continuous media]

Commercial FEM eigenvalue implementations do not incorporate dispersion

EIGENMODE METHOD FAILS IN HIGHLY DISPERSIVE SYSTEMS
Quality factor definition (2): the **eigenmode** and the **field distribution** methods

1. The **eigenmode** method
   - Complex eigenvalue $\tilde{\omega} = \omega' + j\omega''$
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   - Spatial exponential divergence! $\propto \exp\{+r\omega''/c\}$

   ![Diagram of eigenmode method](image1)

   Radial Distance

   $|E|$ for radial distance $r$

   $W$ and $P_{\text{loss}}$ diverge but $W/P_{\text{loss}}$ is constant

   $P_{\text{rad}} + P_e = 2\omega''W - P_{\text{res}}$  

   *(L. D. Landau, *Electrodynamics of continuous media*)

2. The **field distribution** method
   - Driven harmonic simulation @ $\omega_0 = \omega'$
   - Physically incorporates dispersion
   - Spatial and temporal mode decay

   ![Diagram of field distribution method](image2)

   Radial Distance

   $|E|$ for radial distance $r$

   $W$ depends on the integration window

   $W/P_{\text{loss}}$ diverges with radius

**Commercial FEM eigenvalue implementations do not incorporate dispersion**

**EIGENMOMENT METHOD FAILS IN HIGHLY DISPERSIVE SYSTEMS**

**FIELD DISTRIBUTION METHOD REQUIRES CAREFUL CHOICE OF THE INTEGRATION WINDOW**
Alternative approaches: the *eigenfrequency* and the *spectral response* method

3. The *eigenfrequency* method

- Complex eigenvalue $\tilde{\omega} = \omega' + j\omega''$

$$Q = \frac{\omega'}{2\omega''}$$

Commercial FEM eigenvalue implementations do not incorporate dispersion

**EIGENFREQUENCY METHOD FAILS IN DISPERSIVE SYSTEMS**
Alternative approaches: the *eigenfrequency* and the *spectral response* method

3. The *eigenfrequency* method
   - Complex eigenvalue $\tilde{\omega} = \omega' + j\omega''$
   
   $$Q = \frac{\omega'}{2\omega''}$$

Commercial FEM eigenvalue implementations do not incorporate dispersion

4. The *spectral response* method
   - Driven harmonic simulation @ frequencies around $\omega_0$
   
   $$Q = \frac{\omega_0}{\Delta\omega}$$
Alternative approaches: the *eigenfrequency* and the *spectral response* method

3. The *eigenfrequency* method
   - Complex eigenvalue $\tilde{\omega} = \omega' + j\omega''$
   
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4. The *spectral response* method
   - Driven harmonic simulation @ frequencies around $\omega_0$
   
   $$Q = \frac{\omega_0}{\Delta\omega}$$

Commercial FEM eigenvalue implementations do not incorporate dispersion

**EIGENFREQUENCY METHOD FAILS IN DISPENSIVE SYSTEMS**

**SPECTRAL RESPONSE METHOD IS ALWAYS CORRECT**
Application range of the methods via examples
Study examples

Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic $Q$

- Weak dispersion
- Absence of ohmic loss
Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic Q

Study examples

- Weak dispersion
- Absence of ohmic loss

\[ Q_i = \frac{\sqrt{a}}{1 - a} \frac{(2\pi R)\pi n_g}{\lambda_m} \]

[Bogaerts, Laser Photonics Rev. 6, 47, 2012]
[Pendry, Science 312, 1780, 2006]
Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic Q

- Weak dispersion
- Absence of ohmic loss

\[ Q_i = \frac{\omega'}{2\omega''} \]

**Study examples**

\[ \bar{\omega}/2\pi = 193.5 + j0.0085 \text{ THz} \]

Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic $Q$

Study examples

- Weak dispersion
- Absence of ohmic loss

$$Q_i = \omega_0 \frac{W}{P_{rad}}$$
Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic Q

- Weak dispersion
- Absence of ohmic loss

\[ Q_i' = \omega_0 \frac{W}{P_{\text{rad}}} \]
Silicon slab ring resonator @ Near Infrared spectrum // Intrinsic $Q$

- Weak dispersion
- Absence of ohmic loss

$$Q'_i = \omega_0 \frac{W}{P_{rad}}$$
Silicon slab ring resonator @ Near Infrared spectrum // External and Loaded $Q$

- Weak dispersion
- Absence of ohmic loss
Silicon slab ring resonator @ Near Infrared spectrum // External and Loaded $Q$

- Weak dispersion
- Absence of ohmic loss

$\omega/2\pi = 193.5 + j0.0139$ THz

$Q_e = \frac{\omega}{2\omega''}$
Silicon slab ring resonator @ Near Infrared spectrum // External and Loaded $Q$

- Weak dispersion
- Absence of ohmic loss

\[ Q_{\ell} = \omega_0 \frac{W}{P_{rad} + P_c} \]
Silicon slab ring resonator @ Near Infrared spectrum // External and Loaded $Q$

- Weak dispersion
- Absence of ohmic loss

$$Q_L = \frac{\omega_0}{\Delta\omega}$$
Silicon slab ring resonator @ Near Infrared spectrum // External and Loaded $Q$

- Weak dispersion
- Absence of ohmic loss

$$Q_e = \frac{\omega_0}{\Delta \omega}$$

$$T = \frac{4(\omega/\omega_0 - 1)^2 + (1/Q_i - 1/Q_e)^2}{4(\omega/\omega_0 - 1)^2 + (1/Q_i + 1/Q_e)^2}$$

[H. A. Haus, Waves and Fields in Optoelectronics]
Graphene tube resonator @ Far Infrared (THz) spectrum

- Strong dispersion
- Absence of radiation
Graphene tube resonator @ Far Infrared (THz) spectrum

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Study examples

$$Q_i = \omega_0 \frac{W}{P_{res}}$$

$$W = \frac{1}{4} \int \varepsilon_0 \varepsilon \|\mathbf{E}\|^2 \, dr + \frac{1}{4} \int \mu_0 \|\mathbf{H}\|^2 \, dr$$
Graphene tube resonator @ Far Infrared (THz) spectrum

- Strong dispersion
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\[ Q_i = \omega_0 \frac{W}{P_{\text{res}}} \]

\[ W = \frac{1}{4} \int_V \varepsilon_0 \frac{\partial \varepsilon_r(\omega)}{\partial \omega} |E|^2 \, dr + \frac{1}{4} \int_V \mu_0 |H|^2 \, dr + \frac{1}{4} \int_V \frac{\partial \text{Im}\{\sigma(\omega)\}}{\partial \omega} |E|^2 \, dr \]

[Christopoulos, Phys. Rev. E 94, 062219, 2016]
Graphene tube resonator @ Far Infrared (THz) spectrum

- Strong dispersion
- Absence of radiation

\[
Q_i = \omega_0 \frac{W}{P_{\text{res}}}
\]

\[
W = \frac{1}{4} \int_V \varepsilon_0 \frac{\partial \{ \omega \varepsilon_r (\omega) \} }{\partial \omega} |E|^2 dr + \frac{1}{4} \int_V \mu_0 |H|^2 dr + \frac{1}{4} \int_V \frac{\partial \text{Im} \{ \sigma (\omega) \} }{\partial \omega} |E|^2 dr
\]

[Christopoulos, Phys. Rev. E 94, 062219, 2016]
Graphene tube resonator @ Far Infrared (THz) spectrum

- **Strong dispersion**
- **Absence of radiation**

\[ Q_i = \omega_0 \frac{W}{P_{res}} \]

\[ W = \frac{1}{4} \int_{V} \varepsilon_0 \frac{\partial\{\varepsilon_\ell(\omega)\}}{\partial\omega} |E|^2 \, dr + \frac{1}{4} \int_{V} \mu_0 |H|^2 \, dr + \frac{1}{4} \int_{V} \frac{\partial\text{Im}\{\sigma(\omega)\}}{\partial\omega} |E|^2 \, dr \]

[Christopoulos, Phys. Rev. E 94, 062219, 2016]
Dielectric rod resonator/metasurface @ Far Infrared (THz) spectrum

- Weak dispersion
- Radiation and ohmic loss
Dielectric rod resonator/metasurface @ Far Infrared (THz) spectrum

- Weak dispersion
- Radiation and ohmic loss

\[ Q_i = \frac{\omega'}{2\omega''} \]

\[ u \frac{J_m'(u)}{J_m(u)} = \frac{H_m^{(1)}(v)}{H_m^{(1)}(v)} \quad u = \tilde{k}_0 n_{\text{LiTaO}_3} R \]

\[ v = \tilde{k}_0 R \]

[J. A. Stratton, *Electromagnetic Theory*]
Dielectric rod resonator/metasurface @ Far Infrared (THz) spectrum

- Weak dispersion
- Radiation and ohmic loss

Study examples
Dielectric rod resonator/metasurface @ Far Infrared (THz) spectrum

- Weak dispersion
- Radiation and ohmic loss

\[
C_{\text{abs}} = \frac{2(m+1)\lambda}{\pi} \frac{1}{4(\omega/\omega_0-1)^2 + (1/Q_{\text{res}} + 1/Q_{\text{rad}})^2}
\]

[Ruan, J. Phys. Chem. C 114, 013901, 2010]
Dielectric rod resonator/metasurface @ Far Infrared (THz) spectrum

- Weak dispersion
- Radiation and ohmic loss

\[ C_{\text{abs}} = \frac{2(m+1)\lambda}{\pi} \frac{(1/Q_{\text{res}})(1/Q_{\text{rad}})}{4(\omega/\omega_0 - 1)^2 + (1/Q_{\text{res}} + 1/Q_{\text{rad}})^2} \]

[Ruan, J. Phys. Chem. C 114, 013901, 2010]

\[ A = \sum_k 4(\omega_k/\omega_0 - 1)^2 + (1/Q_{\text{res},k} + 1/Q_{\text{rad},k})^2 \]

[H. A. Haus, Waves and Fields in Optoelectronics]

Plasmonic core-shell @ Visible spectrum

- Strong dispersion
- Radiation and ohmic loss

Study examples
Plasmonic core-shell @ Visible spectrum

- Strong dispersion
- Radiation and ohmic loss

Study examples
Plasmonic core-shell @ Visible spectrum

- Strong dispersion
- Radiation and ohmic loss

Study examples

- Field distribution including dispersion
- Spectral response

Intrinsic Quality Factor $Q_i$

- $P_{rad}$
- $R_{max}$
- $R_{out}$

Outer Radius $R$ (nm)

- $TM_{10}$
- $TM_{20}$
- $TM_{30}$

Box A
Study examples

Plasmonic core-shell @ Visible spectrum

- Strong dispersion
- Radiation and ohmic loss

- Eigenfrequency
- Eigenmode neglecting dispersion
- Field distribution including dispersion
- Spectral response

Intrinsic Quality Factor $Q_i$

- Outer Radius $R$ (nm)

- $P_{rad}$, $P_{res}$
- silica, metal, cladding
Plasmonic core-shell @ Visible spectrum

- Strong dispersion
- Radiation and ohmic loss

Study examples
Conclusion

Summary

- Presentation of the $Q$-factor calculation in contemporary photonic resonant structures
- Evaluation in four judiciously chosen structures
- In depth examination of their applicability range with commercially available software

Results

- Strong influence of dispersion on the correct calculation of $Q$
- Light leakage also hardens the calculation

[arXiv:1902.09415]
Thank you!

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