Scattering applications and Q-factors

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Q-models and ideas

- Scattering and Q-factors, in the literature [Optics and Plasmons]
- Q-factors based on system-functions.
- Q-factor with respect to current properties.
Examples of scattering areas with Q-factors


2. Properties of local plasmons in metal nanostructures

Scattering against Microspheres

Q-factors in optics and for plasmons often include micro-resonators

High-Q modes

Given a dielectric sphere, in vacuum, there is a class of mode-solutions that are called Whispering-Gallery modes (Rayleigh). E.g. Solve:

\[
\nabla \times \nabla \times \mathbf{E} - k^2 \varepsilon(r) \mathbf{E} = 0.
\]  

(1)

Variable separation into vector-spherical harmonics in TE/TM-modes. The radial dependence \( \Phi \) satisfy:

\[
\partial_r^2 \Phi + \left( k^2 \varepsilon(r) - \frac{\ell(\ell + 1)}{r^2} \right) \Phi = 0
\]

(2)

There exists solutions \( \Phi = J_\ell(k r) \) when \( \varepsilon = \text{const} \) for special values of \( k_{\ell,q} \).

In the case when \( \ell \gg 1 \), we get (TE)

\[
k_{\ell,q} = \frac{1}{a \sqrt{\varepsilon}} (\ell + a_q(\ell/2)^{1/3} - \sqrt{\frac{\varepsilon}{\varepsilon - 1}} + \frac{3a_q}{20} \left( \frac{2}{\ell} \right)^{1/3} + O(\ell^{-2/3})
\]

(3)

where \( a_q \) is the \( q \):th root to the Airy function \( Ai\left(-z\right) \).
\[ |E_{\phi}|^2 \] is shown for Whispering gallery modes. Here \( n \) is the first zero of the Airy function. Ref: Kippenberg, 2004 PhD thesis.
Whispering gallery modes con’t

The Q-factor for the resonator is defined as usual as

\[ Q = \frac{\omega W_{stored}}{P_{diss}} = \tau \omega \] (4)

Furthermore, due to a range of effects the total Q-factor is

\[ Q^{-1} = Q^{-1}_{b-abs} + Q^{-1}_{rad} + Q^{-1}_{surf-scat} + Q^{-1}_{surf-abs} \] (5)

Here \( Q_{b-abs} = \frac{2\pi n_{ref}}{(\alpha \lambda)} \) is bulk absorption. \( \alpha \) is the intensity attenuation factor, \( n_{ref} \) is the refractive index. Here \( Q_{rad} \) is loss due to radiation. Here \( Q_{surf} \) is surface scattering and absorption terms. In certain plasmon-cases we have that \( Q_{rad} \gg Q_{b-abs} \), e.g. metal losses are larger.

The goal is to have as large \( Q \) as possible to store as much energy as possible: [Grudinin 2007] mention 1cm diam, and give \( \tau = 1s \) at \( \lambda = 1\mu m \). \( Q \sim 10^{12} \).
Whispering gallery modes – spheres

There are several references in the area, and efforts to deal with both electric, thermal and quantum-mechanic effects to find the highest possible Q-factor:

- An electrically large object: (theory) 1cm, with $\lambda = 1\mu$m, $\tau = 1$s, $Q = 10^{12}$. (expr $\lambda =780$nm, $Q = 10^{10}$)
- They consider a dielectric perfect crystal sphere of CaF$_2$. Polishing techniques have eliminated surface absorption and scattering, key limitation: bulk-absorption linear and non-linear.
- They show that Rayleigh scattering limits the absorption at room temperature.
- At cryo-temperature: Brillouin scattering and stimulated Raman scattering seems to be the limiting factor.


Borselli et al., 2005, Opt. Express: Beyond Rayleigh scattering limit in high-Q silicon microdiscs: theory and experiment. [Derivations for the disc, $Q \sim 10^6$, limited by surface roughness, Silicon on insulator disc, $\phi = 5\mu m$, $\lambda \sim 1.5\mu m$]
Min et al., Nature 2009, High-Q surface-plasmon-polariton whispering-galley microcavities: \( R_b \sim 11 \mu m, \lambda = [1.52 - 1.57] \mu m. \)
In this case the Q-factor is here defined as [Simulation, JC silver data]

\[ Q^{-1} = Q_{metal}^{-1} + Q_{rad}^{-1} \]  \hspace{1cm} (6)

where \( Q_{rad} \gg Q_{metal} \).

The method (in supplementary material) to estimate the Q-factor is by using the complex eigenvalue associated with the mode. E.g. If \( f \) is the complex eigen-frequency of the mode then (experiment, transmission, SPP-mode)

\[ Q = \frac{\text{Re} f}{2 \text{Im} f} \sim 10^3 \]  \hspace{1cm} (7)

The separation between metal-losses and radiation losses is done by removing the imaginary part of \( \varepsilon_{Ag} \).

Dielectric resonance \( Q \sim 4000 \)
Observations

- The above cases treat $Q$ as a generic measure of a resonance, e.g. a pole in the complex plane.
- All above cases mainly look on resonators.
- There are often a range of effects coming in: absorption, radiation, surface properties, coupling, often each effect is associated with a resonance and a time-scale.
- In the ‘break-through’ cases key aspect of material properties and fundamental quantum-mechanic effects seems to be the limitation, e.g. at cryo-temperature Stimulated-Raman scattering.
- Geometry effects and radiation seems to be weaker than absorption for metals.
Generic properties of local plasmons

Initial theory:
A Q-factor for generic plasmonic resonances in small metal+dielectric (nano-) structures has been derived. [Wang, Shen, Phys Rev 97, 206806, Lett 2006]

- The theory is based on an approximative quasi-static perturbation theory.
- \[ W_{e,m} = (8\pi)^{-1} \int \partial_\omega (\omega \varepsilon') |E|^2 \, dV \]
- \[ W_{e,d} = (8\pi)^{-1} \int \varepsilon_d |E|^2 \, dV, \]
- \[ \int \varepsilon |E|^2 \, dv = 0. \]
- The Q-factor is then predicted to be

\[
Q = \frac{\omega \partial_\omega \varepsilon'_m}{2 \varepsilon''_m}, \quad \varepsilon_m = \varepsilon'_m + j \varepsilon''_m \tag{8}
\]

![Graph showing quality factor vs. photon energy with curves for Ag and Au](image)
The same paper also give insight into the resonance frequency position according to the model.

The result is independent of shape, and dielectric material.

Assumptions: 1) Quasi-static perturbation theory 2) Stored energy = total energy, only within the structure, 3) frequencies well below the bulk plasma frequency of a low-loss metal. 4) That the dielectric is loss-less.

Goal is a high Q, since it leads to stronger local-field enhancement.
Slow plasmon-resonant nanostructures: nano-antennas

[Bozhevolnyi, Opt. Express 15(17) 2007]: Interface-bounded modes between dielectric and metal at the right frequency is here denoted as surface plasmon-polariton modes (SPP): \( \varepsilon = -23.6 + 1.69i \) (Ag), \( \lambda = 0.65\text{nm} \), \( Q = 5 \)

With multiple surfaces these modes interact and slow down.

Incident plane wave at 45° to x-axis. E/M-dipole like fields \( Q \sim 5 \).
Claim of an improved theroy

Feigenbaum, Orenstein Phys. Rev. Let 101(163902) 2008, account for retardation effects for certain cases. But are unclear about how Q is calculated: E.g. From the field distribution.

Using a Au-nano-particle in a co-axial shield cavity, they obtain an interferometer similar phenomena.

\[ Q \sim 6 \] at \( 1.5 \mu m \) for a gold nano-particle with \( a = 30 \text{nm}, \ L = 60 \text{nm} \), and a gold cylinder with \( b = 90 \text{nm} \). Here \( Q = 30 \) is determined from the field distribution. Excitation by a TM\(_0\)-mode. [Drude-model]

[Min 2009], measured \( Q=1376 \) for the disc at \( \lambda = 1.53 \mu m, \ R = 15 \mu m \)
Q-factor theory, observations

- The quasi-static theory of losses depend only on $\varepsilon$ and its derivatives, tend to predict low $Q$-factors in quasi-static regime.

- A wave-guide field distribution, with a Drude model with a bit unclear $Q$-calculation. Probably they use [Jacksson 1999]

\[
Q = \frac{\int \eta |H|^2 + \partial_\omega (\omega \varepsilon') |E|^2 \, dv}{\int \partial_\omega (\omega \varepsilon'') |E|^2 \, dv}
\]  

but here with the dynamic fields. Note that the non-radiation approximation cause $E$ to be the total field.

An initial search indicate that plasmons with the 1972 JC-metal-data and to maximize the lossy-Q factor for arbitrary (small and large) geometry might be an open problem.
Q-factor from system function

[Li+Liang, PIER 2004] Given a system function $H(s)$ approximated in the form

$$H(s) = \sum_n \frac{R_n}{s - s_n}$$

where the pole can be described as $s_n = -\frac{\omega_n}{2Q_n} + j\omega_n$. An inverse Laplace transform give us the corresponding time response

$$h(t) = \sum_n R_n e^{-\frac{\omega_n}{2Q_n} t} e^{-j\omega_n t}$$

We thus see that a pole of any system function can be associated with a Q-factor for a given angular frequency.
Given e.g. a time-harmonic electric field \( \mathbf{E} = \mathbf{E}_0 \text{e}^{j\omega t} \).

A complex angular frequency \( \omega_c = \omega_0 (1 + j\xi) \). The energy in the system decay exponentially, e.g.

\[
W = W_0 \text{e}^{-j\omega_0 \xi t}
\]  

(12)

The rate of decrease is

\[
P_L = -\frac{dW}{dt} = 2\omega_0 \xi W
\]  

(13)

and thus we can define

\[
Q = \frac{\omega_0 W}{P_L} = \frac{1}{2\xi}.
\]

(14)

It thus make sense to think of a complex pole in terms of the Q-factor.
In Li+Liang, 2004, they utilize the above system function to express the Q-factor for the E-field from an antenna system and a scattering system at a given point. Pade-approximations of the model provide after 'stabilization' of the poles the associated Q-factors to each resonance. In their paper they use a 'validation based on Fosters reaction theorem' from [Collin1966] where

\[
Q = \frac{I^H(\omega_0 \partial_\omega X \pm X)I}{I^H(Z + Z^H)I}
\]

(15)

where \(X\) is the reactance matrix.
[Li + Liang 2004] They consider two PEC-cubes, with an incoming plane wave.
Q-factors and resonances

Out of a Pade-representation \([4,4]\) they identify two stable poles 
\(f = 18\text{MHz}, \text{ with } Q = 9.66\) and \(12.8\text{MHz with } Q = 1.3\)
Scattering case

Given an in-coming plane wave $\mathbf{E}_i$ that scatter upon a PEC object $\Omega$. We find the induced currents through e.g. the EFIE-equation

$$\frac{1}{2} \hat{n} \times \mathbf{E}_{tot}|_{\partial \Omega} = 0 = \hat{n} \times \mathbf{E}_i - \hat{n} \times (\nabla \Phi + j \omega \mathbf{A})$$

where $\phi$ and $\mathbf{A}$ are expressed in terms of the induced surface currents. Introducing a suitable basis function we find with $\mathbf{J} \rightarrow \mathbf{I}$ that

$$\mathbf{V} = \mathbf{ZI}$$

where $\mathbf{Z}$ is the MoM impedance matrix. As a difference to earlier discussion we have here that $\mathbf{V}$ is in general known from the incident field.
Observations/Questions, lossless scattering

1. Vandenbosh 2010 expression for $Q(I)$ gives a Q-factor for any scattering current $I$.

2. $Q(I)$ is a measure of the amount of stored energy to the radiated field, and should hence be directly related to properties of the (total) scattered field.

3. The scattering situation, like the excitation case uniquely determines the induced $I$, and clearly

$$Q(I_{scat}) \geq Q(I_{opt}) , \quad Q(I_{excite}) \geq Q(I_{opt}),$$

Does $Q(I_{scat}) \rightarrow Q_{opt}$ for an optimal shape?
What happens when the structure is lossy?
Volume-loss issues

- Q-factors for lossy material: In plasmon-cases the absorption is the dominating effect, e.g.

\[ Q = \frac{2\omega W_{\text{stored}}}{P_r + P_{\text{loss}}} \approx \frac{2\omega W_{\text{stored}}}{P_{\text{loss}}} \tag{18} \]

What does this do to current-optimization problems?
- Can we distinguish between radiation Q and loss Q? Given one current.
- High Q-factors, rather than low Q-factors to obtain strong field localization? How does this connect with the observation that the Q-factor tend to be un-bounded for PEC-systems.
- To realize the current/scattering behavior we can not relay on multi-position feeding, but have to resort to shape-optimization again.
Meaning of Q in a scattering situation

Can we use $Q$ to measure bandwidth of scattering-based quantities. For certain far-field associated information probably. Several scattering-interesting parameters are measured in the far-field. Thus for example, the bandwidth of partial scattering cross section is defined as

$$\frac{\pi}{2} \frac{\partial \Omega \sigma(\omega, \hat{r})}{\partial \omega} = \left| \frac{F(\omega, \hat{r}) Z Q^{-1} \hat{t} \cdot E_0}{k^2|E_0|^2} \right|^2. \tag{19}$$

will depend (among other things) on how rapidly $I$ varies with respect to $\omega$. ($F$ is known, thus we have its explicit frequency behavior).
Comparison – Q-factor

Consider an PEC antenna $\lambda/2 \times \lambda/100@1\text{GHz}$. We can easily compare the $Q$-factors for e.g. the dipole:

![Graph showing Q-factors vs frequency]

- $Q_{\text{opt}}$ in blue
- $Q_{\text{in}}$ in red
- $Q_{\text{scat}}$ in green

Clearly $Q_{\text{opt}} \leq Q_{\text{scat}}$, and $Q_{\text{opt}} \leq Q_{\text{excite}}$.
Comparison – far-field

For a given current (opt, in, excitation) we find the radiated field as

\[ F(\hat{r}) = \sum_{n} f_n(\omega) A_n(\hat{r}) \]  \hspace{1cm} (20)
Empirically the position of the first few resonances for excitation and scattering are similar (for broadside case of a dipole).

Using vector-fit we can derive a model for $f_n$ in scattering and excitation. The graph above indicate that the local complex resonances are similar.

The Q-factor is closely related to the resonance size of $\Gamma$, are $f_n$-similar to $\Gamma$.

Is there a relation between $Q(I)$ and complex resonances, and in such a case how does the relation look like.
A different approach

The Q-factor is based on currents. This provide information about the frequency stability of \( J \).
Can we measure the 'distance' between \( J(\omega) \) and \( J(\omega_0) \) in a reasonable way that involves \( Q \)? ⇒ Using a stored energy norm gets us a partial expression.

\[
\| J(\omega) \|^2_{W(\omega)} - \| J(\omega_0) \|^2_{W(\omega_0)} = \\
(\omega - \omega_0) \left( 2Q \Re \langle \partial_{\omega} J, RJ \rangle + \langle J, \partial_{\omega} W J \rangle \right) + O(\omega - \omega_0)^2 \quad (21)
\]

It is a measure of change between two frequencies, however 1) it depends on \( \partial_{\omega} J \) which we have no information about.