Probing the fundamental detection limit of photonic crystal cavities: supplementary material

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   This document provides supplementary information to "Probing the fundamental detection limit of photonic crystal cavities," https://doi.org/10.1364/optica.4.000757. It consists of two parts: The first one details the different calculation steps that lead to Eq. (2) of the main article, and the second one discusses the perturbation approach carried out in the main article in relation to the one developed by Yang *et al.* in [1].

1. INTRODUCTION

The first purpose of this supplementary materials document is to provide intermediate technical steps that have been implemented to determine Eq. (2) and Eq. (5).

2. CALCULATION STEPS LEADING TO EQ. (2)

Our goal is to express the relative voltage fluctuation $\delta U/U$ in function of the frequency fluctuations $\delta \omega$ of the cavity resonance. The various notations are provided in the primary manuscript. Setting $a = \frac{1}{4Q_i Q_c}$ and $b = \frac{1}{4Q^2}$, where Q_i is the intrinsic cavity quality factor, i.e. the quality factor of the photonic crystal cavity free of any access waveguides, and Q_c the quality factor resulting from the in-plane coupling, the spectral response of the cavity is given by:

$$S(\omega_0, \omega_p) = \frac{a}{((\omega_p - \omega_0)/\omega_0)^2 + b}. \tag{S1}$$

   Introducing the out of plane scattered intensity $I^{scat} = \frac{b}{a} I^{in}$ at zero detuning, i.e. $x = 0$, this last equation can be rewritten as

$$S(\omega_0, \omega_p) = \frac{b}{((\omega_p - \omega_0)/\omega_0)^2 + b} \frac{I^{scat}}{I^{in}}, \tag{S2}$$

   which corresponds to the equation (1) provided in the main article. The fluctuation of the scattered intensity for a given variation of the cavity frequency $\delta \omega$ can be expressed as:

$$\delta I^{scat}/I^{in} = -S(\omega_0, \omega_p) + S(\omega_0 + \delta \omega, \omega_p). \tag{S3}$$

   Using $x = (\omega_p - \omega_0)/\Delta \omega$ as defined in the main article, provides a simplified expression of the two following quantities that are involved in the development of Eq. (S3):

$$\left(\frac{\omega_p - \omega_0}{\omega_0}\right)^2 = 4bx^2, \tag{S4}$$

$$\left(\frac{\omega_p - \omega_0 - \delta \omega}{\omega_0 + \delta \omega}\right)^2 = 4b\frac{x - \delta \omega/\Delta \omega}{1 + \delta \omega/\Delta \omega/Q}. \tag{S5}$$

It follows:

$$\frac{\delta I^{scat}}{I^{in}} = -\frac{1}{1 + 4x^2} + \frac{1}{1 + 4\left(\frac{x - \delta \omega/\Delta \omega}{1 + \delta \omega/\Delta \omega/Q}\right)^2}. \tag{S6}$$

   The intensity that is measured without fluctuations for a given detuning x is $I^{scat}|_x = \frac{1}{4x^2+1} I^{scat}$, which implies:

$$\frac{\delta I^{scat}}{I^{scat}|_x} = -1 + \frac{1 + 4x^2}{1 + 4\left(\frac{x - \delta \omega/\Delta \omega}{1 + \delta \omega/\Delta \omega/Q}\right)^2} = \delta U/U|_{\delta \omega}. \tag{S7}$$

   The last equation corresponds to the equation (2) of the main article since the photo voltage U is proportional to the scattered intensity.

3. CALCULATION STEPS LEADING TO EQ. (5)

We consider that the photonic system is a closed system of volume $\mathcal{V}$, i.e. we neglect any dissipation, which is a good approximation for high-Q cavities. The Helmholtz equation that

governs the electric field $\vec{E}$ of a dielectric cavity whose dielectric map is $\epsilon_c(\vec{r})$, can be written as:

$$\frac{1}{\epsilon_c(\vec{r})}\vec{\nabla} \times \vec{\nabla} \times \vec{E} = \left(\frac{\omega}{c}\right)^2 \vec{E}, \quad \textbf{(S8)}$$

where $\times$ stands here for the vectorial product. Defining the scalar product as $<\vec{E}|\vec{E}> = \iiint_V \epsilon_c(\vec{r})\vec{E}(\vec{r})\vec{E}^*(\vec{r})d\vec{r}$, this last equation can be written with an Hermitian operator $\hat{\Theta}_E \vec{E} = \lambda_0 \vec{E}$ where $\lambda_0 = (\omega/c)^2$. The symbol * stands for the complex conjugate. When a nanoparticle is present in the surrounding of the cavity the dielectric map is modified as $\epsilon(\vec{r}) = \epsilon_c(\vec{r}) + \delta\epsilon(\vec{r})$ where $\delta\epsilon(\vec{r})$ is the local perturbation induced by the nanoparticle. Writing $1/(\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r}))$ as

$$\frac{1}{\epsilon_c(\vec{r})} - \frac{1}{\epsilon_c(\vec{r})} + \frac{1}{\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r})} = \frac{1}{\epsilon_c(\vec{r})} - \frac{\delta\epsilon(\vec{r})}{\epsilon_c(\vec{r})(\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r}))}, \quad \textbf{(S9)}$$

the perturbed Helmholtz equation becomes:

$$\frac{1}{\epsilon_c(\vec{r})}\vec{\nabla} \times \vec{\nabla} \times \vec{E} - \frac{\delta\epsilon(\vec{r})}{\epsilon_c(\vec{r})(\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r}))}\vec{\nabla} \times \vec{\nabla} \times \vec{E} = \left(\frac{\omega}{c}\right)^2 \vec{E}. \quad \textbf{(S10)}$$

Defining the perturbation operator $\hat{V}_{perturb}$ as

$$\hat{V}_{perturb} = \frac{\delta\epsilon(\vec{r})}{\epsilon_c(\vec{r})(\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r}))}\vec{\nabla} \times \vec{\nabla} \times, \quad \textbf{(S11)}$$

Eq. (S10) takes the operational form: $(\hat{\Theta}_E + \hat{V}_{pert})\vec{E} = \lambda_{pert}\vec{E}$ where the eigenvalue λ_{pert} can be written as $\lambda_{pert} = \lambda_0 + \delta\lambda_{pert}$

From standard perturbation theory:

$$\delta\lambda_{pert} = \frac{<\vec{E}|\hat{V}_{perturb}|\vec{E}>}{<\vec{E}|\vec{E}>} = -\lambda_0 \frac{\int \frac{\epsilon_c(\vec{r})\delta\epsilon(\vec{r})}{\epsilon_c(\vec{r}) + \delta\epsilon(\vec{r})}|\vec{E}(\vec{r})|^2 dV}{\int \epsilon_c(\vec{r})|\vec{E}(\vec{r})|^2 dV}. \quad \textbf{(S12)}$$

Considering that the dielectric perturbation cancels, $\delta\epsilon = 0$, except in the spatial domain defined by the nanoparticle of volume V_{part}, and assuming that the field amplitude is constant over the nanoparticle, the perturbation part of the operator eigenvalue is

$$\delta\lambda_{pert} = -\lambda_0 \frac{\delta\epsilon(\vec{R})}{\epsilon_c(\vec{R}) + \delta\epsilon(\vec{R})} \frac{V_{part}}{V_{eff}} \frac{\epsilon_c(\vec{R})|\vec{E}(\vec{R})|^2}{max\{\epsilon_c(\vec{r})|\vec{E}(\vec{r})|^2\}}, \quad \textbf{(S13)}$$

where the effective mode volume of the cavity is defined as $V_{eff} = \frac{\int \epsilon_c(\vec{r})|\vec{E}(\vec{r})|^2 dV}{max\{\epsilon_c(\vec{R})|\vec{E}(\vec{R})|^2\}}$. With our definition of the scalar product, it follows that:

$$\delta\lambda_{pert} = -\lambda_0 \frac{\delta\epsilon(\vec{R})}{\epsilon_c(\vec{R}) + \delta\epsilon(\vec{R})} \frac{V_{part}}{V_{eff}} \frac{<\vec{E}|\vec{E}>|_{\vec{r}=\vec{R}}}{max\{<\vec{E}|\vec{E}>\}}. \quad \textbf{(S14)}$$

Using the notations $||E_{part}||^2 = <\vec{E}|\vec{E}>|_{\vec{r}=\vec{R}}$ and $||E_{max}||^2 = max\{<\vec{E}|\vec{E}>\}$, and the first order development $\delta\lambda_{pert} = \delta\omega^2 \approx 2\omega_0\delta\omega$, we retrieve the equation of the main article.

$$\frac{\delta\omega}{\omega_0}|_{pert} = -\frac{1}{2}\frac{\delta\epsilon}{\epsilon_c + \delta\epsilon}\frac{V_{part}}{V_{eff}}\frac{||E_{part}||^2}{||E_{max}||^2}. \quad \textbf{(S15)}$$

Note that the notations $||E_{part}||^2$ and $||E_{max}||^2$ stand for the field intensity according to our definition of the scalar product and should not be confused with the modulus of the fields $|E_{part}|^2$ and $|E_{max}|^2$, more specifically $||E_{part}||^2 = \epsilon_c(\vec{R})|E_{part}|^2$.

Our purpose now is to make contact between the approach that has been developed in [1] and the closed system approximation. Using quasi-normal mode (QNM) $(\vec{E}, \vec{H})$ with a complex-valued eigenfrequency $\tilde{\omega}$, the frequency shift induced by a perturbation of volume V_p has been determined in [1]:

$$\frac{\delta\tilde{\omega}}{\tilde{\omega}} = -\frac{\iiint_{V_p} \delta\epsilon(\vec{r}, \tilde{\omega})\vec{E}'(\vec{r}) \cdot \vec{E}(\vec{r})d^3\vec{r}}{\iiint_\Omega \left\{\vec{E} \cdot \frac{\partial[\omega\epsilon(\vec{r},\omega)]}{\partial\omega}\vec{E} - \vec{H} \cdot \frac{\partial[\omega\mu(\vec{r},\omega)]}{\partial\omega}\vec{H}\right\}d^3\vec{r}}, \quad \textbf{(S16)}$$

where $\vec{E}'$ represents the quasi normal mode dressed by the perturbation and the volume Ω can be chosen as the entire space. The tilde symbol highlights the complex value of the wave vector of the QNM.

In analogy with the effective mode volume, a generalized mode volume can be defined as:

$$\tilde{V} = \frac{\iiint_\Omega \left\{\vec{E} \cdot \frac{\partial[\omega\epsilon(\vec{r},\omega)]}{\partial\omega}\vec{E} - \vec{H} \cdot \frac{\partial[\omega\mu(\vec{r},\omega)]}{\partial\omega}\vec{H}\right\}d^3\vec{r}}{2\{\epsilon\vec{E} \cdot \vec{E}\}}, \quad \textbf{(S17)}$$

where $\{\epsilon\vec{E} \cdot \vec{E}\}$ is taken at the position that corresponds to $max\{\epsilon_c(\vec{r})|\vec{E}(\vec{r})|^2\}$. When the imaginary part of the wave vector vanishes, i.e. when the system can be considered as a close system, the generalized mode volume $\tilde{V}$ becomes identical to V_{eff}. With the definition of $\tilde{V}$, Eq. S16 can be expressed as:

$$\frac{\delta\tilde{\omega}}{\tilde{\omega}} = -\frac{1}{2}\frac{V_p}{\tilde{V}}\frac{1}{V_p}\frac{\iiint_{V_p} \delta\epsilon(\vec{r}, \tilde{\omega})\vec{E}'(\vec{r}) \cdot \vec{E}(\vec{r})d^3\vec{r}}{\{\epsilon\vec{E} \cdot \vec{E}\}}. \quad \textbf{(S18)}$$

An approximation based on a local-field correction is carried out in [1] to expressed the dressed electric field $\vec{E}'$ in term of the unperturbed electric field $\vec{E}$. As a result, using our current notations and $V_p = V_{part}$, the complex frequency shift for a spherical nano particle is given by:

$$\frac{\delta\tilde{\omega}}{\tilde{\omega}} = -\frac{1}{2}\frac{\delta\epsilon(\vec{R})}{\epsilon_c(\vec{R}) + \delta\epsilon(\vec{R})/3}\frac{V_{part}}{\tilde{V}}\frac{\epsilon_c(\vec{R})\vec{E}(\vec{R}) \cdot \vec{E}(\vec{R})}{\{\epsilon\vec{E} \cdot \vec{E}\}}. \quad \textbf{(S19)}$$

Such an expression is similar to the one obtained for a closed system, see Eq. S15, except the factor $1/3$ in the denominator of the fraction $\delta\epsilon(\vec{R})/(\epsilon_c(\vec{R}) + \delta\epsilon(\vec{R})/3)$. Instead of the approximation implemented in [1], we suggest to take $\vec{E}' = \epsilon_c(\vec{R})\vec{E}/\epsilon(\vec{R})$, which leads to:

$$\frac{\delta\tilde{\omega}}{\tilde{\omega}} = -\frac{1}{2}\frac{\delta\epsilon(\vec{R})}{\epsilon_c(\vec{R}) + \delta\epsilon(\vec{R})}\frac{V_{part}}{\tilde{V}}\frac{\epsilon_c(\vec{R})\vec{E}(\vec{R}) \cdot \vec{E}(\vec{R})}{\{\epsilon\vec{E} \cdot \vec{E}\}}. \quad \textbf{(S20)}$$

When the imaginary part of the wave vector tends to zero, this last equation allows the expected convergence of the frequency shift toward the one obtained for a closed system.

Note that writing $\vec{E}' = \epsilon_c(\vec{R})\vec{E}/\epsilon(\vec{R})$ is equivalent to set the equality of the perturbed and unperturbed electric displacement fields at the position of the perturbation.

Finally, the two approaches differ mainly in the definition of the mode volume. For high-Q cavities the effective mode volume V_{eff} is a good approximation whereas for strongly leaky modes V_{eff} has to be replaced by the generalized mode volume as defined by Eq. S17.

4. CONCLUSION

This supplementary materials document adds extra information to support the results achieved in the main article entitled "Probing the fundamental detection limit of photonic crystal cavities," Optica volume 4, first page 757 (2017). We have detailed all the calculation steps that are necessary to retrieve Eq. (2) and to relate $\delta I^{scat}/I_{in}$ and $\delta U/U$ as defined in section 3 of the main manuscript. Furthermore, we have discussed the Eq. (5) of the main manuscript in view of the model developed in [1]. We have highlighted the differences and similarities between our approach leading to Eq. (5) and the approach followed by Yang et al. This comparison suggests modifying an approximation made by Yang et al. in order to make contact between these two approaches.

REFERENCES

1. J. Yang, H. Giessen, P. Lalanne, Nano Lett. **15**, 3439-3444 (2015).