Maximization of the Quality Factor of an Optical Resonator

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Abstract

We consider resonance phenomena for the scalar wave equation in an inhomogeneous medium. Resonance is a solution to the wave equation which is spatially localized while its time dependence is harmonic except for decay due to radiation. The decay rate, which is inversely proportional to the qualify factor, depends on the material properties of the medium. In this work, the problem of designing a resonator which has high quality factor (low loss) is considered. The design variable is the index of refraction of the medium. High quality resonators are desirable in a variety of applications, including photonic band gap devices.

Finding resonance in a linear wave equation with radiation boundary condition involves solving a nonlinear eigenvalue problem. The magnitude of the ratio between real and imaginary part of the eigenvalue is proportional to the quality factor Q. The optimization we perform is finding a structure which possesses an eigenvalue with largest possible Q. We present a numerical approach for solving this problem. The method consists of first finding a resonance eigenvalue and eigenfunction for a non-optimal structure. The gradient of Q with respect to index of refraction at that state is calculated. Ascent steps are taken in order to increase the quality factor Q. We demonstrate how this approach can be implemented and present numerical examples of high Q structures.

1 Introduction

This work is motivated by recent research in photonic band gap devices. Photonic band gap refers to the existence of frequency bands in which no light can propagate. This effect can be realized in an infinite medium whose dielectric constant is spatially periodic [20, 11]. When a defect is introduced into such a medium, it is possible to create standing waves which are localized near the defect [7, 12]. A defect mode can be exploited in different applications.

Lossless defect modes exist only in theory since medium of infinite extents is an idealization. When a photonic band gap medium is finite, waves can escape from the structure to the surrounding medium. Interestingly, one is still able to create fields which are localized. However, due to the losses to radiation, instead of a standing wave of constant amplitude, one is left with a standing wave whose amplitude decays in time. Such a solution to the time-dependent wave equation is called a *resonance*.

Resonance calculations for the wave equation involve finding a solution whose behavior is not physical but approximates well the time dependent nature of the resonance phenomenon [10, 13]. Consider the initial value problem for the 1-D time-dependent Schrödinger's

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equation

$$u_{tt} = u_{xx} - V(x)u, \quad -\infty < x < \infty,$$

and initial conditions

$$u(x,0) = u_0, \quad u_t(x,0) = u_1.$$

We assume that the potential satisfies $V(x) = 0$ for $|x| \geq x_0$, and that $V(x)$ has a well at the origin. Then energy will be trapped by the well, but because the well has finite wall thickness, energy tunnels out of the well and radiates to infinity. Therefore, the system loses energy.

To solve this problem, one recasts the problem in finite domain and apply radiation boundary conditions

$$\begin{aligned} &u_{tt} = u_{xx} - V(x)u, \quad |x| < x_0, \\ &u_x - u_t = 0, \ \ x = -x_0, \\ &u_x + u_t = 0, \ \ x = x_0. \end{aligned}$$

We seek a solution of the form $u(x,t) = \varphi(x)e^{-i\omega t}$, which leads us to consider

$$\begin{aligned} &-\varphi'' + V(x)\varphi = \omega^2\varphi, \quad |x| < x_0, \\ &\varphi' + i\omega\varphi = 0, \ \ x = -x_0, \\ &\varphi' - i\omega\varphi = 0, \ \ x = x_0. \end{aligned}$$

Solutions to this problem are found for a countable number of complex ω, denoted here by $\{\omega_n\}$, with the following property [13]

$$\omega_n = i\alpha_n - \beta_n, \quad \text{where } \alpha_n < 0.$$

The ordering is $\alpha_{n+1} \leq \alpha_n$. The eigenfunctions, are referred to as 'quasi normal modes', while their eigenvalues are called resonances. Note that $\varphi_n(x)$ grows exponentially

$$\varphi_n(x) \sim e^{-\alpha_n|x|},$$

so they are non-physical. Never-the-less, we have the following estimate [13]. Choose t_0, a, b, and ϵ. Then there exist a constant C depending on t_0, a, b, and ϵ such that

$$\left| u(x,t) - \sum_{n=1}^{N} A_n e^{(\alpha_n + i\beta_n)t}\varphi_n(x) \right| \leq Ce^{(-|\alpha_{N+1}|+\epsilon)t},$$

holds for every $t > t_0$, and $a < x < b$. This means that after some time, the solution is well described by a superposition of (non-physical) modes that oscillate at frequency β_n die away exponentially in time at the rate of α_n. In particular, if we have an eigenvalue ω_n such that $|\alpha_n|$ is very small, the solution behaves like a damped standing wave after large times.

We note another way to characterize these quasi-normal modes is by looking at the spectral problem

$$-\varphi'' + V(x)\varphi = \omega^2\varphi, \quad x \in \mathbb{R},$$

with $V(x)$ as previously described. For any real ω, we can write two linearly independent solutions to the differential equation. We can in fact write the Green's function as products of these solutions divided by the Wronskian in the usual way. The resonance corresponds to values of ω for which the Wronskian vanishes. This happens when we continue the Wronskian into the complex plane. The quasi-normal mode can be identified as one of the solutions (which are linearly dependent) of the differential equation at this value of ω.

The subject of this paper is to create a medium which is efficient at trapping waves; i.e., a good resonator. That is, we seek a medium which has a resonance $\omega_n = i\alpha_n - \beta_n$ with very small $|\alpha_n|$. To give a measure of the decay, we use the notion of quality factor Q. It is defined as the ratio between total energy stored and the energy dissipated per cycle. We can understand this concept by studying a damped mass-spring system, whose motion $x(t)$ is governed by [14]

$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0^2 x = 0, \tag{1}$$

where $\gamma > 0$ and ω_0 is the natural frequency. The general solution of this second-order ordinary equation for small damping ($\frac{\gamma}{\omega_0} \ll 1$) is

$$x(t) = Ae^{-\gamma t}\cos(\omega_1 t + \delta),$$

where $\omega_1 = \sqrt{\omega_0^2 - \gamma^2}$ is the damped frequency and δ is the phase shift. The constants A and δ are uniquely determined by the initial conditions. Since the total energy

$$E(t) = \frac{1}{2}\left[\frac{dx(t)}{dt}\right]^2 + \frac{1}{2}\omega_0^2[x(t)]^2,$$

and the period is $T = 2\pi/\omega_1$, we easily find that

$$E(T) = E(0)e^{-2\gamma t}.$$

The quality factor

$$\begin{aligned} Q &= 2\pi\frac{\text{Total energy stored at beginning of the cycle}}{|\text{Energy lost during a cycle}|} \\ &\cong 2\pi\frac{E(0)}{E(0) - E(T)} = 2\pi\frac{1}{1 - e^{-2\gamma\frac{2\pi}{\omega_1}}} \cong \frac{\omega_1}{2\gamma}\ . \end{aligned}$$

The independent solutions of (1) are of the form $e^{i\omega t}$ where $\omega = \pm\omega_1 + i\gamma$. Therefore an alternate interpretation for Q is

$$Q \cong \frac{1}{2}\left|\frac{\text{Real part of } \omega}{\text{Imaginary part of} \omega}\right|. \tag{2}$$

This simple derivation illustrates how we compute the quality factor for a damped mass-spring system. The energy loss here is due to the mechanical damping which shows up in the imaginary part of ω. If there is little damping, i.e. γ is small, Q is high.

For the wave equation, the quality of a resonator Q can be defined in exactly the same manner as that for the damped oscillator. That is, if the medium possesses quasi-normal modes, each of these modes has a quality factor Q which is one half the real part of the complex eigen frequency divided by the imaginary part. In this paper, we are interested in designing a medium, that is, a distribution of the material properties in that medium in order to achieve a high quality for a particular mode. We devise a gradient ascent method for the procedure by starting from an initial medium. The medium is then changed iteratively, each time improving the quality factor of a mode. Each iteration involves computation of the quality factor and its gradient with respect to the medium. These involve solution of a nonlinear eigenvalue problem, which could be quite large depending on the size of the medium and the wavelength of the eigenfunction. In Section 2, we decribe a way to find the quasi normal modes and resonances. We show how to calculate the gradient of the quality Q with respect to the material property in Section 3. The gradient allows us to formulate an algorithm for maximizing Q, which we describe in Section 4. In Section 5, we give numerical simulations to illustrate our approach. The paper ends with a discussion section. An appendix contains a discussion of the one-dimensional problem which exhibits special features.

2 Resonance calculation via integral equation

The method we describe below can be applied to resonance problems in any dimension, and for Maxwell's equations. However, we will focus the discussion to a two-dimensional scalar wave problem. Consider Helmholtz's equation

$$\Delta u + \omega^2(1+\rho(x))u = 0, \quad x \in \mathbb{R}^2. \tag{3}$$

The medium, which is inhomogeneous, is characterized by the function $\rho(x)$, which we assume to satisfy $0 \leq \rho(x) \leq \rho_+$. That is, we assume that the material with which we construct has index of refraction greater than that of air. Moreover, $\rho(x)$ is supported inside a bounded region Ω. It can be seen that ρ is the square of the index of refraction. Throughout this paper, we may refer to ρ as the index.

The field u satisfies the Sommerfeld radiation boundary condition

$$\lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u}{\partial r} - i\omega u\right) = 0. \tag{4}$$

Since (4) is not a local boundary condition, (3) with this boundary condition is not a standard boundary value problem. One can replace the radiation condition with an approximate absorbing boundary condition such as the Engquist-Majda [6] boundary condition, the perfectly matched layer (PML) [3], or a truncated Dirichlet-to-Neumann series [8]. Applying any of these conditions with (3) turns the problem into a boundary value problem from which the quasi-normal modes can be determined. Here we choose an alternate approach.

The Green's function for the scalar wave equation in a homogeneous infinite medium satisfies

$$\Delta G + \omega^2 G = \delta(x-y).$$

In two dimensions, we have

$$G(\omega, x) = -\frac{i}{4}H_0^1(\omega|x|),$$

where H_0^1 is the Hankel function of the first kind. It is clear that $G(\omega, x)$ satisfies the Sommerfeld radiation condition. We can now rewrite the solution to (3)–(4) in integral form

$$u(x) + \omega^2 \int_\Omega G(\omega, x-y)\rho(y)u(y)dy = 0. \tag{5}$$

To find the quasi-normal modes, we seek values of ω in (5) that yield nontrivial solutions $u(x)$. This problem can be seen as a nonlinear eigenvalue problem since the 'eigenvalue' ω appears not only as a multiplier but also in the kernel $G(\omega, \cdot)$. One can also see that the eigenvalue must be complex by multiplying the equation with complex conjugate of $u(x)$ and integrating over Ω. We will also have use for the left quasi-normal mode defined by the equation

$$v(x) + \omega^2 \rho(x) \int_\Omega G(\omega, x - y) v(y) dy = 0. \tag{6}$$

Next, we will discretize the equations.

In order to compute the convolution in the integral term efficiently, we use the Fast Fourier Transform (FFT). Since the integral term has weak singularity, a corrected trapezoidal quadrature rule, described below, will be used to take this into account. The domain $\Omega = [0, 2\pi]^2$ is discretized with equal spaced points (x_p, x_q) with $p, q = 0, 1, 2, ..., N$, $x_j = hj$ and $h = 2\pi/N$.

Define the operator $A(\omega)$ as

$$A(\omega)u = u(x) + \omega^2 \int_\Omega G(\omega, x - y)\rho(y)u(y)dy, \tag{7}$$

and its adjoint operator $A^*(\omega)$ is

$$A^*(\omega)v = v(x) + \omega^2 \rho(x) \int_\Omega G(\omega, x - y)v(y)dy. \tag{8}$$

The Green's function $G(\omega, x)$ has a logarithmic singularity at $x = 0$

$$G_\omega(x) \sim \frac{1}{2\pi} \ln x + \frac{1}{2\pi}(\ln \frac{\omega}{2} + 0.5772156649015328606) - \frac{i}{4}.$$

Thus, special care must be taken when applying a quadrature rule to evaluate the integrals above.

The discrete approximations of $A(\omega)$ and $A^*(\omega)$ in (7) and (8) by the trapezoidal rule are

$$[A_h(\omega)u]_{p,q} = u(x_p, x_q) + \omega^2 h^2 \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s} \rho(x_r, x_s) u(x_r, x_s), \tag{9}$$

and

$$[A_h^*(\omega)v]_{p,q} = v(x_p, x_q) + \omega^2 h^2 \rho(x_p, x_q) \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s} v(x_r, x_s). \tag{10}$$

The function $g(\omega)_{p,q}$ in (9)–(10) are samples of the Green's function when it is regular, and corrected versions to take into account the weak singularity when $p = q = 0$. The correction is devised to obtain $O(h^4)$ accuracy in the integration when the function integrated against $G(\omega, x - y)$ is smooth [1, 2]. The function $g(\omega)_{p,q}$ is given by

$$g(\omega)_{p,q} = \begin{cases} -\frac{i}{4} + \frac{1}{2\pi}\left(\ln(h\omega/2) + \gamma + c_1\right) & \text{if} \quad (p,q) = (0,0) \\ -\frac{i}{4} H_0^1(\omega\sqrt{x_p^2 + x_q^2}) & \text{if} \quad p^2 + q^2 > 0 \end{cases},$$

with $\gamma = 0.5772156649015328606$ and $c_1 = -1.2133459579012365$.

Given $\rho(x)$, we have a nonlinear eigenvalue problem

$$A_h(\omega)u = 0, \tag{11}$$

to solve for eigenvalues ω and eigenfunctions u. A classical method for solving the nonlinear eigenvalue problem is the inverse iteration. It amounts to applying Newton's method to solve a system of nonlinear equations [16].

The inverse iteration finds one eigenvalue starting with an initial guess for the eigenfunction. We will need the derivative of the operators $A_h(\omega)$ and $A_h^*(\omega)$ with respect to ω, which we denote by $A_h'(\omega)$ and $A_h^{*\prime}(\omega)$. We can solve for both the left and right eigenvectors simultaneously. The iterative process is as follows. For $s = 0, 1, 2, \cdots$,

1. Solve for $\tilde{u}_h^{(s+1)}$ and $\tilde{v}_h^{(s+1)}$ in

$$A_h(\omega^{(s)})\tilde{u}_h^{(s+1)} = A_h'(\omega^{(s)})u_h^{(s)},$$
$$A_h^*(\omega^{(s)})\tilde{v}_h^{(s+1)} = A_h^{*\prime}(\omega^{(s)})v_h^{(s)}.$$

2. Update the eigenvalue according to

$$\omega^{(s+1)} = \omega^{(s)} - \frac{(\tilde{v}_h^{(s+1)})^T A_h(\omega^{(s)})\tilde{u}_h^{(s+1)}}{(\tilde{v}_h^{(s+1)})^T A_h'(\omega^{(s)})\tilde{u}_h^{(s+1)}}.$$

3. Normalize according to

$$u_h^{(s+1)} = \frac{\tilde{u}_h^{(s+1)}}{\|\tilde{u}_h^{(s+1)}\|}, \qquad v_h^{(s+1)} = \frac{\tilde{v}_h^{(s+1)}}{\|\tilde{v}_h^{(s+1)}\|}.$$

We need to obtain a good initial guess for the inverse iterations. To do this we start by choosing a frequency ω_0 which is close to the desired frequency of the quasi-normal mode. Then we solve the linear eigenvalue problem

$$-h^2 \sum_{r,s=0}^{N-1} g(\omega_0)_{p-r,q-s}\rho(x_p, x_q)u(x_p, x_q) = \frac{1}{\omega^2}u(x_p, x_q),$$

for eigenpairs (ω, u). We then pick the eigenvectors u whose eigenvalue is closest to ω_0 and set this as the initial guess for $u^{(0)}$. Let us denote this eigenvalue by ω_0^*. The initial guess for the right eigenvector $v^{(0)}$ is obtained by solving the linear system

$$0 = v(x_p, x_q) + (\omega_0^*)^2 h^2 \rho(x_p, x_q) \sum_{r,s=0}^{N-1} g(\omega_0)_{p-r,q-s} v(x_r, x_s).$$

There is absolutely no guarantee that the inverse iterations will yield an eigenvalue close to ω_0, although we do observe this in our computations.

We note that we do not need to explicitly evaluate the matrices corresponding to $A_h(\omega)$ and $A_h^*(\omega)$. Instead, we use the FFT to evaluate their action of given vectors through (9)–(10). This fact leads us to use generalized minimal residual (GMRES) [9] to solve the linear systems involved in Step 1 of the inverse iterations.

In the inverse iteration, we need to compute the derivative of $A(\omega)$ with respect to ω. We use the definition of the operator in (7) and differentiate both sides to obtain

$$\frac{\partial A(\omega)u}{\partial \omega} = 2\omega \int G(\omega, x-y)\rho(y)u(y)dy + \omega^2 \int G_\omega(\omega, x-y)\rho(y)u(y)dy.$$

Here $G_\omega(\omega, x) = \frac{i}{4}H_1^1(\omega|x|)|x|$. We note that

$$G_\omega(\omega, 0) = \frac{1}{2\pi\omega},$$

which is not singular. Therefore we can use the FFT and regular trapezodial rule to compute the second integral term. We have

$$\begin{aligned}[A_h'(\omega)u]_{p,q} &= 2\omega h^2 \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s}\rho(x_r, x_s)u(x_r, x_s) \\ &+\omega^2 h^2 \sum_{r,s=0}^{N-1} g'(\omega)_{p-r,q-s}\rho(x_r, x_s)u(x_r, x_s),\end{aligned} \tag{12}$$

where

$$g'(\omega)_{p,q} = \begin{cases} \frac{1}{2\pi\omega} & \text{if} \quad (p,q) = (0,0) \\ \frac{i}{4}H_1^1(\omega\sqrt{x_p^2 + x_q^2})\sqrt{x_p^2 + x_q^2} & \text{if} \quad p^2 + q^2 > 0 \end{cases}.$$

A similar expression is derived for $A_h^{*\prime}(\omega)$. We now have all the ingredients needed to perform the inverse iterations to calculate a quasi-normal mode given a medium, described by $\rho(x)$.

We note that the calculation can proceed in a similar way in three dimensions. The calculation is a little more involved if one is to consider Maxwell's equation. For the 1-D problem, exact absorbing boundary conditions are local. We find that the quasi-normal mode calculation in this case amounts to a quadratic eigenvalue problem. We discuss this in detail in the Appendix.

3 Q-factor maximization

The procedure by which the Q-factor is optimized is as follows. We start with a medium $\rho(x)$ and calculate a quasi-normal mode associated with the medium. Then we proceed by changing $\rho(x)$ in order to increase the Q-factor associated with that quasi-normal mode. The medium is assumed to satisfy $0 \le \rho(x) \le \rho_+$. We note that this is not a rigorous optimization but rather it is a continuation method. The difficulty in posing a mathematically correct optimization problem associated with eigenvector optimization has been pointed out in [5]. Indeed the computational method described here is fashioned after that described in [5].

In order to devise a maximization method, we need to calculate the gradient of the Q-factor with respect to the medium $\rho(x)$. The basic method to do this is a perturbational calculus. Consider the nonlinear eigenvalue problem (11) involved in finding a quasi-normal mode

$$A_h(\omega, \rho)u = 0.$$

We have explicitly denoted the dependence of the operator A_h on ω and ρ; its dependence is described in (9). Suppose the pair (ω, u) satisfy the above nonlinear equation. Next we introduce a small perturbation to the medium $\delta\rho$. What we want to know is how ω and u change under this perturbation.

We can formally write the following

$$A_h(\omega + \delta\omega, \rho + \delta\rho)(u + \delta u) = 0.$$

Expanding and keeping only first order terms in the expansion we get

$$\left[A_h(\omega, \rho) + A_h'(\omega, \rho)\delta\omega + \delta A_h(\omega)\right](u + \delta u) \approx 0. \tag{13}$$

Here we denote by $\delta A_h(\omega)$ the change in the matrix $A_h(\omega, \rho)$ caused by the perturbation $\delta\rho$. Upon further expansion, and again keeping only first order terms, we obtain

$$A(\omega, \rho)\delta u + \delta\omega A_h'(\omega, \rho)u + \delta A_h(\omega)u = 0.$$

Let v be the left eigenvector satisfying

$$A_h^*(\omega, \rho)v = 0, \quad \text{or} \quad v^T A_h(\omega, \rho) = 0.$$

See (10) for the definition of the adjoint operator. Then, Multiplying (13) by v^T and rearranging, we get

$$\delta\omega = -\frac{v^T\, \delta A_h(\omega)\, u}{v^T\, A_h'(\omega, \rho)\, u}. \tag{14}$$

This equation shows how a nonlinear eigenvalue changes when the matrix is perturbed. This perturbational problem has been studied in [18].

Our interest is in the Q-factor. Recall from (2) the definition of Q, which we rewrite as

$$Q = -\frac{i(\omega + \overline{\omega})}{2(\omega - \overline{\omega})}.$$

If the eigenvalue is perturbed by $\delta\omega$, the Q-factor perturbation is

$$\delta Q = i\frac{(\overline{\omega}\delta\omega - \omega\overline{\delta\omega})}{(\omega - \overline{\omega})^2}. \tag{15}$$

Having obtained the expression for how Q changes as the material ρ is perturbed by $\delta\rho$, we can proceed to obtain a formula for the gradient of Q with respect to ρ.

We note that from (9) we can calculate

$$[\delta A_h(\omega)u]_{p,q} = \omega^2 h^2 \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s}\delta\rho(x_r, x_s)u(x_r, x_s).$$

We can now fill in the formula for $\delta\omega$ in (14). Let

$$\begin{aligned}
B &= v^T\, A_h'(\omega, \rho)\, u \\
&= 2\omega^2 h^2 \sum_{p,q=0}^{N-1} \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s}\rho(x_r, x_s)u(x_r, x_s)\overline{v(x_p, x_q)} \\
&+\omega^2 h^2 \sum_{p,q=0}^{N-1} \sum_{r,s=0}^{N-1} g'(\omega)_{p-r,q-s}\rho(x_r, x_s)u(x_r, x_s)\overline{v(x_p, x_q)}.
\end{aligned}$$

The value of B is known as soon as we have found the right and left eigenvectors u and v. The formula for $\delta\omega$ is

$$\delta\omega = \frac{1}{B}\omega^2 h^2 \sum_{p,q=0}^{N-1} \sum_{r,s=0}^{N-1} g(\omega)_{p-r,q-s} \delta\rho(x_r, x_s) u(x_r, x_s) \overline{v(x_p, x_q)}. \tag{16}$$

Thus, given $\delta\rho$, one can easily calculate $\delta\omega$ from (16). Let us define

$$K_{r,s} = \frac{1}{B}\omega^2 h^2 \sum_{p,q=0}^{N-1} g(\omega)_{p-r,q-s} u(x_r, x_s) \overline{v(x_p, x_q)}, \tag{17}$$

so that we can write

$$\delta\omega = \sum_{r,s=0}^{N-1} K_{r,s} \delta\rho(x_r, x_s).$$

Let us rewrite δQ in (15) as

$$\delta Q = \frac{-i}{4(\mathrm{Im}\omega)^2} \left(\overline{\omega}\delta\omega - \omega\overline{\delta\omega} \right).$$

Combining this with the last expression for $\delta\omega$ leads to

$$\delta Q = \frac{-i}{4(\mathrm{Im}\omega)^2} \sum_{r,s=0}^{N-1} \left[\overline{\omega} K_{r,s} - \omega \overline{K_{r,s}} \right] \delta\rho(x_r, x_s).$$

From this expression, we make the identification that the formal gradient of Q with respect to the medium is

$$[\mathrm{grad}Q]_{r,s} = \frac{-i}{4(\mathrm{Im}\omega)^2} \left[\overline{\omega} K_{r,s} - \omega \overline{K_{r,s}} \right], \tag{18}$$

where $K_{r,s}$ is given in (17). We note that the terms on the right-hand side produce a real number since $[\overline{\omega} K_{r,s} - \omega \overline{K_{r,s}}]$ is imaginary.

We can now devise a simple steepest ascent algorithm to increase Q:

1. Begin with a medium ρ.
2. Find a quasi-normal mode u and the left eigenvector v.
3. Calculate quality factor Q and its gradient grad$Q$.
4. Update $\rho \leftarrow \rho + \tau\, \mathrm{grad}Q$.
5. Project candidate ρ so that it falls in the interval $[0, \rho_+]$.
6. Return to step 2.

As we iterate, we note that not only the medium ρ changes, the resonance frequency ω and the quasi-normal mode also changes. If we take τ sufficiently small, we should be able to track the same resonance through the iterations, and that Q will be increased at each step.

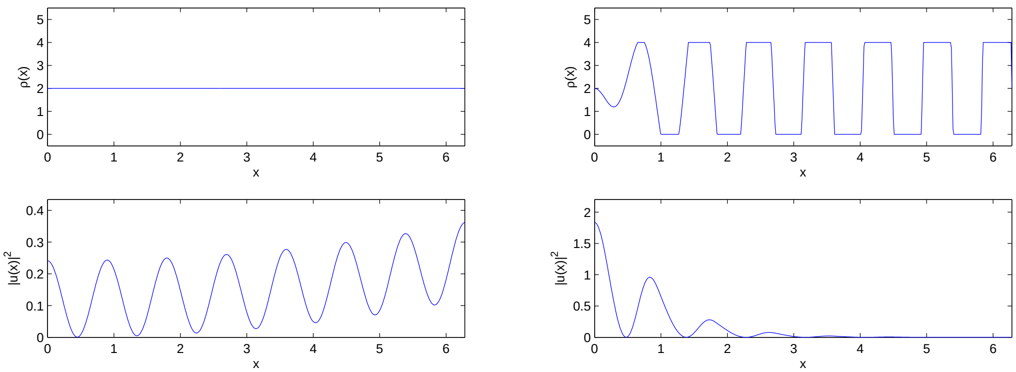

Figure 1: On the left is the initial index profile and the absolute value squared of a quasi-normal mode with eigenvalue $\omega = 2.0209 - 0.0605i$. This mode is optimized for large Q. The maximized profile is shown on the right. It possesses a quasi-normal mode with eigenvalue $\omega = 2.0215 - 7.2877 \times 10^{-5} i$; the absolute value squared of the quasi-normal mode is shown.

4 Numerical examples

We begin with 1-D calculations. For simplicity, we seek quasi-normal modes which are symmetric about $x = 0$. The integral equation is, c.f. (5)

$$u(x) + \omega^2 \int_0^L G(\omega, x, y)\rho(y)u(y)dy = 0.$$

We seek ω such that the above yields a nontrivial solution satisfying $u(0) = 0$. The index $\rho(x)$ is supported in the interval $[0, L]$. The Green's function is simply

$$G(\omega, x, y) = \begin{cases} -\frac{i}{2\omega}\left(e^{i\omega y} + e^{-i\omega y}\right)e^{i\omega x} & x > y > 0 \\ -\frac{i}{2\omega}\left(e^{i\omega x} + e^{-i\omega x}\right)e^{i\omega y} & 0 < x < y \end{cases}.$$

Alternatively, we could use the formulation presented in the Appendix and solve for the eigenmodes of a non-self-adjoint two-point boundary value problem.

In each of the experiment, we take $L = 2\pi$ and start with $\rho = 2$. We also require $0 \leq \rho(x) \leq 4$. A quasi-normal mode near a given frequency is calculated. In Figure 1 (left), we show plots of $\rho(x)$ and the absolute value squared of a quasi-normal mode, $|u(x)|^2$, whose eigenvalue is $\omega = 2.0209 - 0.0605i$. The mode can be interpreted as a resonance with frequency 2.0209 and decay rate of 0.0605. We remind the reader that this is a quasi-normal mode, which is not physical. This fact can be seen by the growth of the mode amplitude as x increases.

We apply the maximization algorithm described in Section 4. The index profile shown in Figure 1 (right) is the result of the maximization, and shown below it is the quasi-normal mode amplitude squared. The frequency of this resonance has shifted slightly to 2.0215 while the decay rate has been reduced to 7.2877×10^{-5}. Notice that the resulting medium consists of a periodic structure with a 'defect' near $x = 0$. The quality factor associated with this resonance is $Q = 1.3870 \times 10^4$.

In the second example, we look for a resonance with a higher frequency. The medium shown in Figure 2 (left) supports a resonance with frequency 2.8872 and decay rate 0.0605.

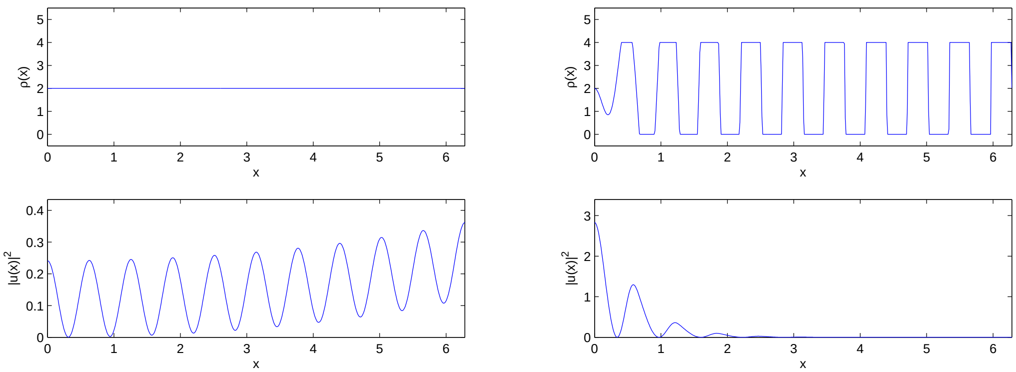

Figure 2: On the left is the initial index profile and the absolute value squared of a quasi-normal mode with eigenvalue $\omega = 2.8872 - 0.0605i$. The maximized profile is shown on the right. It possesses a quasi-normal mode with eigenvalue $\omega = 2.9085 - 1.7973 \times 10^{-6}i$; the absolute value squared of the quasi-normal mode is shown.

The quasi-normal mode associated with this resonance is shown. The maximized profile is given on the right, with the associated quasi-normal mode shown below. The resonance frequency has shifted to 2.9085 while the decay rate has been reduced to 1.7973×10^{-6}. The quality factor associated with this resonance is $Q = 8.0914 \times 10^5$.

In two dimensions, we face the computational challenge of large problem size. To resolve a wave, it is desirable to have at least 12 to 15 points per wavelength. The structure we are seeking varies at the scale of 1/4 to 1/2 the wavelength. Together, these requirements force us to consider low frequency resonances (relative to the domain size). The domain on which the index $\rho(x, y)$ is allowed to vary is chosen to be the square $[0, 2\pi]^2$. In the two experiments we present, the initial distribution is a constant $\rho(x, y) = 3$. We require $0 \leq \rho(x, y) \leq 5$. Two quasi-normal modes are calculated for this material distribution, one with eigenvalue $\omega = 1.0245 - 0.0824i$, and the other, with eigenvalue $\omega = 1.2092 - 0.0584i$.

Figure 3 summarizes the result of the first 2-D calculation. The left column shows the index distribution $\rho(x, y)$ at various stages of optimization, while the right column shows the associated quasi-normal modes. The white parts on the left column are of value 5 while the black part are of value 1. The quasi-normal modes have been normalized so that they are of the same norm within the 2π-by-2π domain to emphasize the localization effects. As can be seen from the figure, the larger the quality factor Q, the more localized the mode. The final eigenvalue is $\omega = 1.4340 - 0.0022$, showing that the frequency has shifted slightly from its initial value. What is more significant is that the imaginary part has been made smaller, giving $Q = 321.95$. The quality factor of the initial, constant medium was $Q = 6.2158$.

Next we considered the problem of maximizing Q for a slightly higher frequency resonance. With the initial index of set at $\rho(x, y) = 3$, we considered a quasi-normal mode with eigenvalue $\omega = 1.2092 - 0.0584i$, and quality factor $Q = 20.71$. The results of our computation is summarized in Figure 4. Displayed again are $\rho(x, y)$ and $|u(x, y)|^2$ at various stages of maximization. The maximized resonance has $Q = 2136.98$, corresponding to frequency 1.5211 and decay rate 0.0007. In both cases, the optimized media are lace-like structures. We conjecture that had we done the computation on a finer mesh and maximized a higher frequency mode, the resulting medium will resemble a photonic bandgap structure – periodic

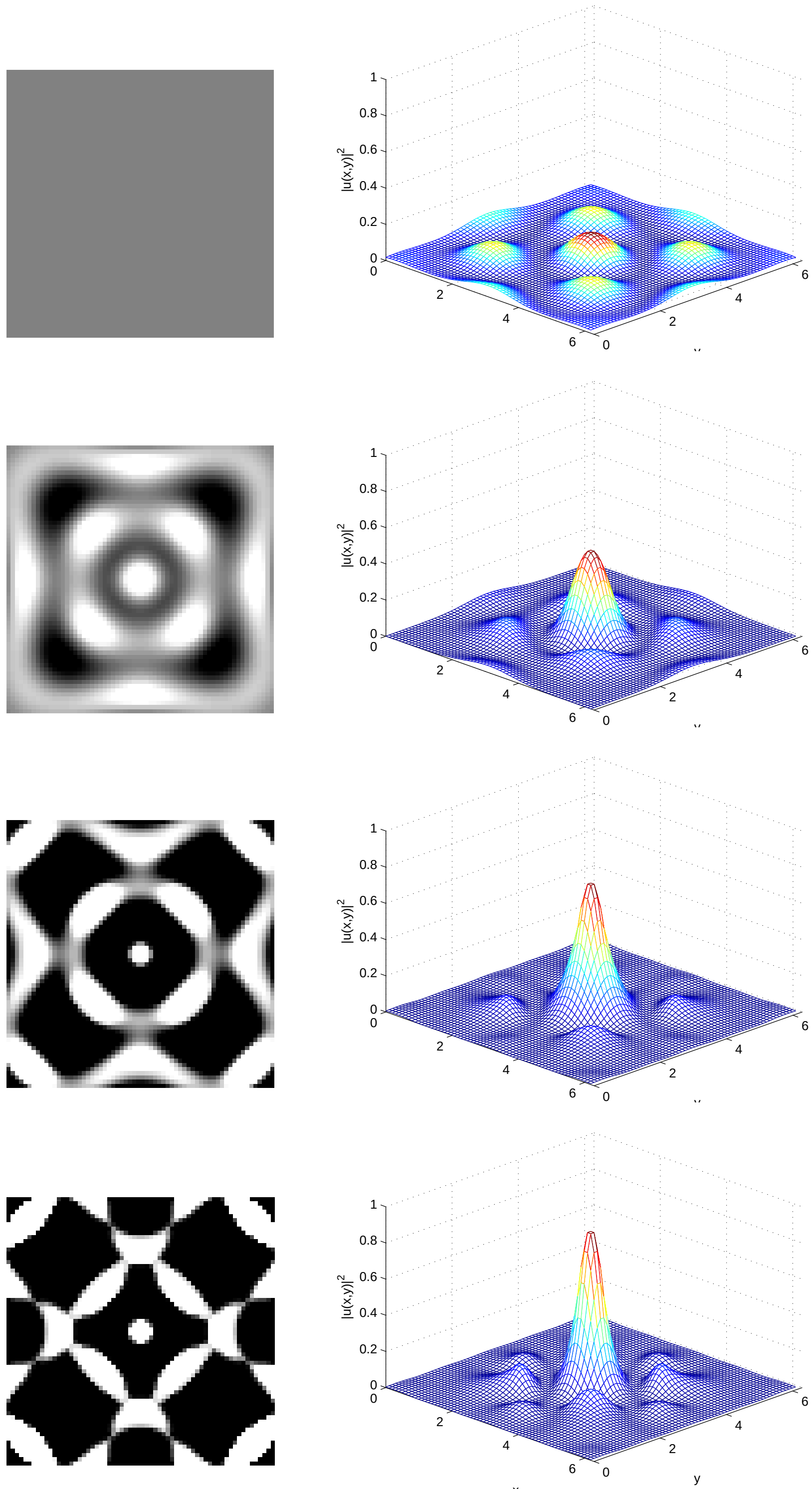

Figure 3: The column on the left displays the index distribution $\rho(x, y)$ through the maximization steps (black=5, white=0). The distribution is initially set to $\rho(x, y) = 3$. The column on the right shows the absolute value squared of the quasi-normal mode being maximized. Note that high Q mode is very localized. The mode being maximized started with resonance frequency 1.0245 and decay rate 0.08241. After maximization, the frequency is 1.4340, whereas the decay rate has been reduced to 0.0022, resulting in $Q = 321.15$.

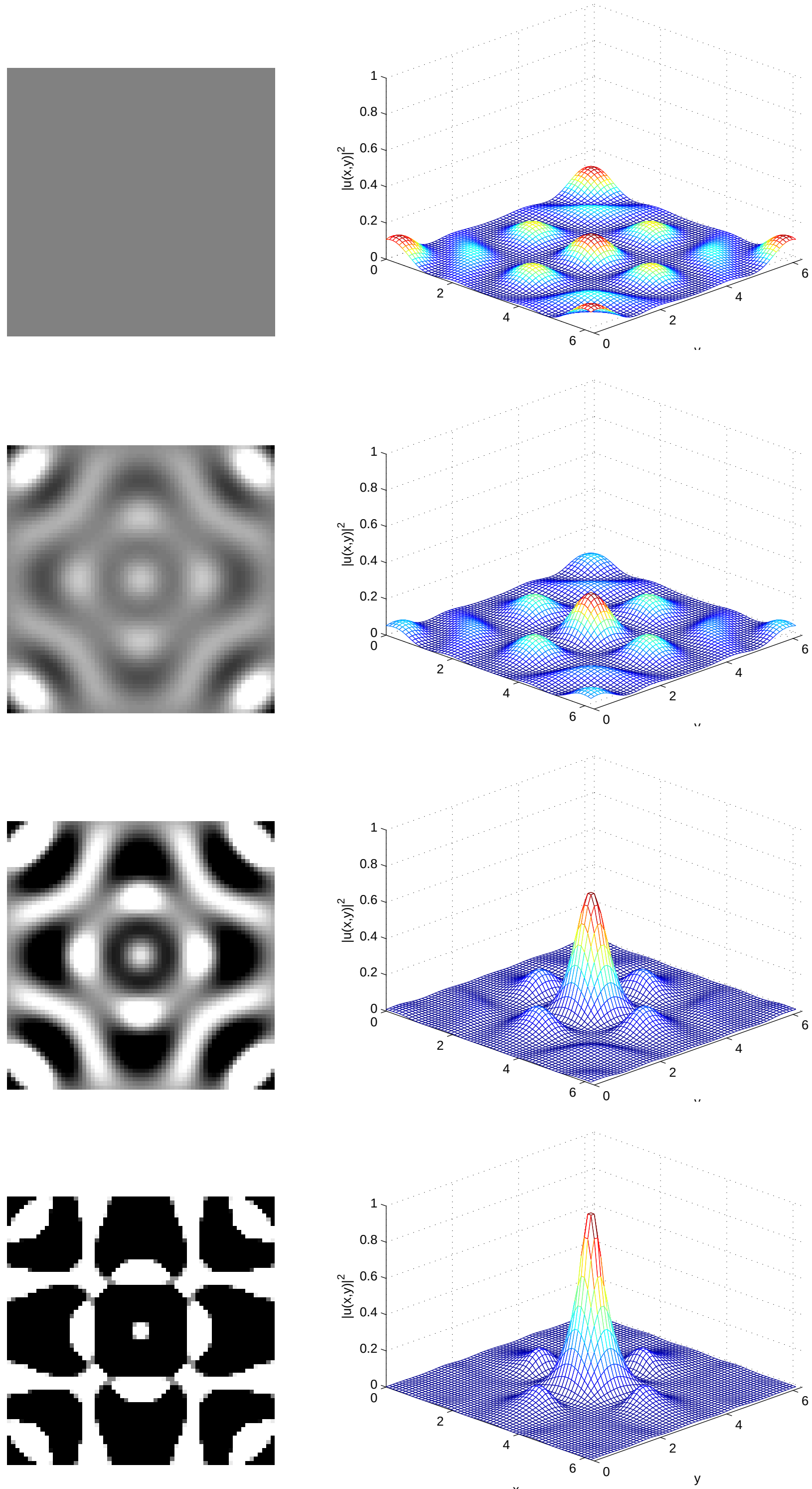

Figure 4: In this example, we maximize Q for a slightly higher frequency resonance. The column on the left displays the index of distribution $\rho(x, y)$ through the maximization steps (black=5, white=0). The distribution is initially set to $\rho(x, y) = 3$. The column on the right shows the absolute value squared of the quasi-normal mode being maximized. The mode being maximized started with resonance frequency 1.2092 and decay rate 0.0584. After maximization, the frequency is 1.5211, whereas the decay rate has been reduced to 0.0007, resulting in $Q = 2136.98$.

medium with a defect.

We note that a medium may admit multiple (nonlinear) eigenvalues. We have observed that as maximization steps are taken, the quasi-normal mode that is being followed as the medium changes may become one of two (or more) quasi-normal modes with the *same* eigenvalue. When the process encounters such a point, it is not capable of determining which quasi-normal mode to follow. We provided a 'fix' for such a situation in the case of eigenvalue maximization [5]. Unfortunately the remedy does not work for the present situation because we are calculating only a single quasi-normal mode at each step of the iteration. One idea may be to take a step that is in the direction of increasing Q but at the same time, the resulting quasi-normal mode after updating the medium should not differ too much from the one in the previous iteration. This added complication in the computation is beyond the scope the present work.

5 Discussion

We present a computational method for designing an optical resonator which has high quality factor, Q. Optical resonance is achieved by creating a medium with variable index of refraction. The quality factor is calculated from the resonance frequency associated with a quasi-normal mode. We start with a known structure and a quasi-normal mode whose quality factor we would like to improve. We devise a continuation method which 'follows' the particular quasi-normal mode as the medium is changed. We take steps in the gradient direction of Q with respect to the medium to ensure that Q is increased.

Both 1-D and 2-D numerical results are provided. In 1-D our method produces a medium which resembles a periodic structure with a defect. In 2-D it produces lace-like structures. We were able to perform 2-D computations only for low frequency resonance because of the computational resource limitation. We are confident that very efficient 2-D resonators can be created using our method. It is clear that calculations in 3-D, and those using vector Maxwell equation, will require enormous computational resources. This fact points to the need for more efficient ways of modeling the wave phenomena, which may be achieved perhaps through the use of asymptotics [15]. Finally, we observed that Q is large when the quasi-normal mode is highly localized. This seems to indicate that one may not need to optimize Q through resonance calculation. It might be possible that we can obtain good designs by ignoring the radiation boundary condition and just simply look for a bounded medium which supports a highly localized eigenmode, as done in [5].

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Appendix: Resonances for the 1-D wave equation

Consider the time-dependent 1-D wave equation for $U(x,t)$

$$(1+\rho(x))\,U_{tt} - U_{xx} = 0, \quad x \in \mathbb{R}.$$

The function $\rho(x)$ satisties $0 \le \rho \le \rho_+$ and is zero for $|x| \ge L$. We wish to study resonances of this system. We can put the problem in a finite domain by using the radiation boundary condition at $x = \pm L$

$$U_t(\pm L, t) \pm U_x(\pm L, t) = 0.$$

This is because we have explicitly assumed that $\rho(x) = 0$ for $|x| \ge L$, and no energy can propagate towards the origin from $|x| > L$. To find resonances, we consider solutions of the type $U(x,t) = u(x)e^{-i\omega t}$. Therefore, $u(x)$ satisfies

$$u'' + \omega^2(1 + \rho(x))u = 0, \tag{19a}$$
$$u'(-L) + i\omega u(-L) = 0, \tag{19b}$$
$$u'(L) - i\omega u(L) = 0. \tag{19c}$$

We now seek eigenvalues ω such that the above system yields a nontrivial solution $u(x)$. The eigenfunctions $u(x)$ are the quasi-normal modes. Note that this is a nonlinear eigenvalue problem as the differential equation and the boundary conditions depend on ω.

There are several ways we can solve this eigenvalue problem. We adopt the finite element method [17]. First, we derive the weak formulation by multiplying (19b) with an smooth test function $v(x)$ and integrating by parts to obtain

$$v(L)u'(L) - v(-L)u'(-L) - \int_{-L}^{L} u'(x)v'(x)dx + \omega^2 \int_{-L}^{L} (1 + \rho(x))\, u(x)v(x)dx = 0.$$

Apply the boundary conditions (19c)–(19c) to get

$$\begin{aligned} &-i\omega\, [v(L)u(L) + v(-L)u(-L)] \\ &\quad - \int_{-L}^{L} u'(x)v'(x)dx + \omega^2 \int_{-L}^{L} (1 + \rho(x))\, u(x)v(x)dx = 0. \end{aligned} \tag{20}$$

Next we discretize the problem by representing the solution as a linear combination of piecewise linear finite element basis

$$u(x) = \sum_{j=1}^{n} u_j \phi_j(x).$$

We use a regular mesh for convenience as discretize the interval $[-L, L]$ into $(n-1)$ equal subintervals of size $h = 2L/(n-1)$. We label $x_1 = -L$, $x_2 = -L + h$, ..., $x_n = L$, and scale $\phi_j(x)$ such that they take on the value of 1 at these mesh points. As usual $\phi_j(x) = 0$ for $x \le x_{j-1}$ and $x \ge x_{j+1}$. The coefficients u_j represent the values of $u(x)$ at the mesh points x_j.

Substituting the approximation in (21) gives us

$$\begin{aligned} &-i\omega[v(L)u_n + v(-L)u_1] \\ &\quad - \sum_{j=1}^{n} u_j \int_{-L}^{L} v'(x)\phi_j'(x)dx + \omega^2 \sum_{j=1}^{n} u_j \int_{-L}^{L} (1 + \rho(x))v(x)\phi_j(x)dx = 0. \end{aligned}$$

We choose the test function $v(x)$ from the set of basis functions $\phi_j(x)$. Therefore we arrive at

$$
\begin{aligned}
&-i\omega[\phi_k(L)u_n + \phi_k(-L)u_1] - \sum_{j=1}^{n} u_j \int_{-L}^{L} \phi_k'(x)\phi_j'(x)dx \qquad (21)\\
&+\omega^2 \sum_{j=1}^{n} u_j \int_{-L}^{L} (1+\rho(x))\phi_k(x)\phi_j(x)dx = 0, \quad \text{for } k = 1, 2, \ldots, n.
\end{aligned}
$$

Defining the mass matrix M by

$$M_{jk} = \int_{-L}^{L} (1+\rho(x))\phi_k(x)\phi_j(x)dx,$$

the stiffness matrix K by

$$K_{jk} = \int_{-L}^{L} \phi_k'(x)\phi_j'(x)dx,$$

and the damping matrix by

$$C = -\begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{bmatrix}.$$

Then (22) can be written as

$$\left(\omega^2 M + i\omega C - K\right) u = 0, \qquad (22)$$

which is a quadratic eigenvalue problem involving n-by-n matrices. This problem is easily reduced to the familiar generalized eigenvalue problem

$$\left[\begin{pmatrix} 0 & I \\ -K & C \end{pmatrix} - i\omega \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix}\right] \begin{pmatrix} u \\ i\omega u \end{pmatrix} = 0. \qquad (23)$$

Given $\rho(x)$, this can be easily solved by existing eigenvalue solvers.

Denote

$$\Theta(\omega) = \omega^2 M + i\omega C - K.$$

Since $\Theta(\omega)^* = \Theta(-\bar{\omega})$, the distribution of the eigenvalues of $\Theta(\omega)$ in the complex plane is symmetric with respect to the imaginary axis. This is also true for the distribution of eigenvalues (1) in the mass-spring system. If u is a right eigenvector associated with the eigenvalue ω, then u is a left eigenvector associated with the eigenvalue $-\bar{\omega}$ [19].

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