Quasi-normal modes and the resonant response of open phononic systems

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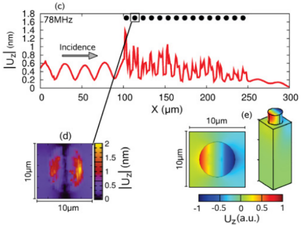
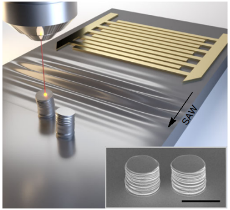
Physical motivation

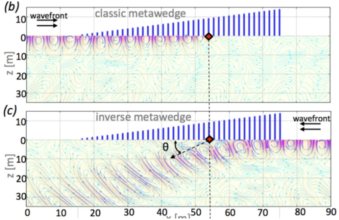
- There are many systems in phononics that deal with discrete resonators in interaction with a radiation substrate
- Following ideas from photonics/plasmonics, can we use the concept of quasi-normal mode (QNM) to predict their response?



Achaoui et al., PRB 2011
10.1103/PhysRevB.83.104201



Raguin et al., Nat. Commun. 2019
10.1038/s41467-019-12492-z



Colombi et al., Sci Reports 2016
10.1038/srep27717

A short nomenclature of modes in wave physics

- A **closed** finite resonator sustains **normal modes**
- An **open** finite resonator sustains **quasi-normal modes**
  - If there is coupling to radiation modes, we speak of a **resonance**,
  - If there is no coupling, then we speak of **bound states in the continuum (BIC)**. BIC is lossless (real eigenfrequency) and often originates from a symmetry different from continuum waves
- If there is an invariance axis, a waveguide can be formed [examples: optical waveguides, optical fibers, surface acoustic waves, Rayleigh / Love waves in geophysics]
  - Outside the light or sound cone (where there are no propagating bulk waves), there are (evanescent) **guided waves**,
  - Inside the cone, there are either resonances (also termed **leaky waves**) or BICs!
- The same concepts and terms are used for **crystal waveguides** (that are periodic along a given direction)

Normal modes

- Normal modes are eigenmodes of *closed* structures
- Mathematically, for elastic waves they are the eigensolutions of

$$\omega_n^2 \rho(\omega_n) \mathrm{u}_n = -\nabla \cdot (c(\omega_n) : \nabla \mathrm{u}_n) \tag{1}$$

  with exterior boundary conditions (typically free or clamped)
- In the absence of loss, eigenfrequencies ω_n are real and eigenvectors u_n are orthogonal
- The total energy of normal modes is bounded

$$H(\mathrm{u}_n) = \frac{1}{2}\left(\int S_n^* : c(\omega) : S_n + \omega_n^2 \int \mathrm{u}_n^* \cdot \rho(\omega) \mathrm{u}_n\right) < \infty \tag{2}$$

$$S_n = \nabla \mathrm{u}_n \tag{3}$$

Quasinormal modes (QNMs)

- Quasi-normal modes (QNMs) are eigenmodes of *open* structures, suffering radiation to infinity
- They satisfy the same equation as normal modes

$$\omega_n^2 \rho(\omega_n) \mathrm{u}_n = -\nabla \cdot (c(\omega_n) : \nabla \mathrm{u}_n) \qquad (4)$$

but with outgoing-wave boundary conditions at infinity and with $\omega_n \in \mathbb{C}$

- Quality factor: $Q_n = \frac{\Re \omega_n}{2 \Im \omega_n}$
- Their total energy is unbounded (similar to leaky modes of waveguides)

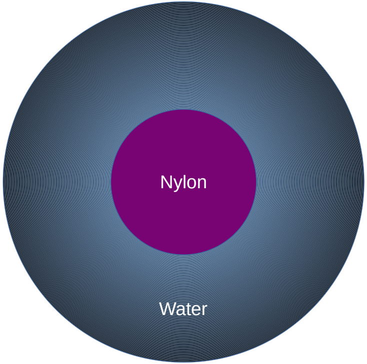
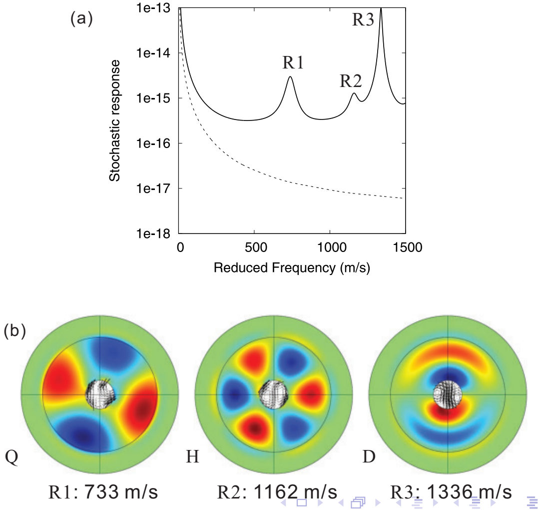


Figure: A nylon rod immersed in (infinite) water. What are its mechanical eigenmodes?

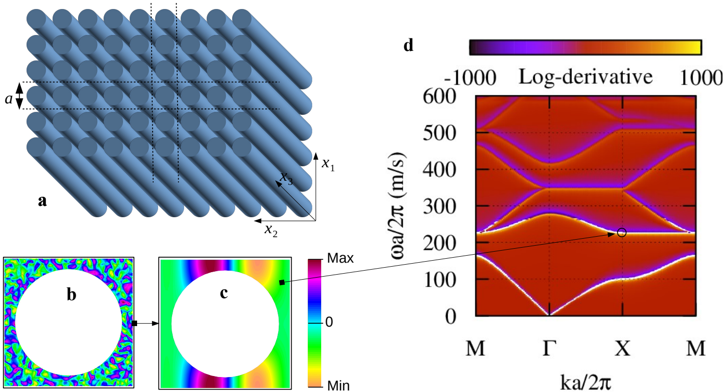
Response function and poles

- We can also solve for the frequency response (with the PML) and observe poles
  Laude & Korotyaeva, Phys. Rev. B **97**, 224110 (2018)
- Maxima give approximately the real part of the eigenfrequency
- The peak width gives a quality factor Q
- Resonant response gives approximately the QNM!
- Example: Y. F. Wang, S. Y. Zhang, Y. S. Wang, & V. Laude, Phys. Rev. B **102** 144303 (2020)



Stochastic excitation technique to obtain the resolvent band structure

- Physical idea: local excitations of the system result in resonances. Spatially random excitation garanties none are forgotten
  Laude & Korotyaeva, Phys. Rev. B **97**, 224110 (2018)



How can we obtain QNMs? There are 2 basic ways...

1. The beautiful and heroic way: Green's function techniques
   - Use some approximation in the finite region (e.g. FEM), couple it to the exterior analytic solution (plane waves in 1D, Bessel/Hankel functions in 2D, spheroidal harmonics in 3D)
   - Example: M. B. Doost, W. Langbein, and E. A. Muljarov. "Resonant-state expansion applied to three-dimensional open optical systems." Physical Review A **90** 013834 (2014).
2. The 'ugly' and efficient way: replace the infinite radiation medium with a perfectly matched layer (PML)
   - Use some eigenvalue solver to obtain the complex eigenmodes of the now 'closed' system
   - Example: C. Sauvan, J. P. Hugonin, I. S. Maksymov, and P. Lalanne. Theory of the spontaneous optical emission of nanosize photonic and plasmon resonators. Physical Review Letters **110** 237401 (2013).

Beware, it is not as easy as it seems...

PMLs have many 'spurious' eigenmodes, it is difficult to sort QNMs from them!

Definition of computational domains

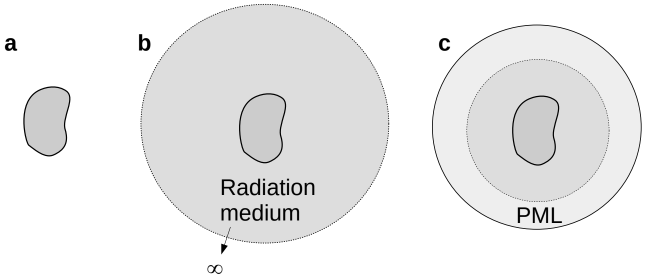
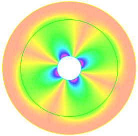


Figure: Definition of supporting domains for wave resonance and propagation. (**a**) Finite, closed domain supports normal modes. (**b**) Infinite, open domain supports quasinormal modes. (**c**) These can be approximated by closing the domain of computation with a perfectly matched layer (PML), that is the truncated image of the infinite domain in (**b**) in a complex coordinate transformation.

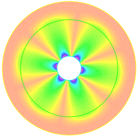
A practical algorithm to obtain one QNM

Start with ω_0 close to a maximum of the response

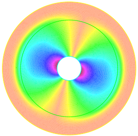
1. Initialization is stochastic: solve $(K - \omega_0^2 M)\mathrm{u}_0 = F$ for random F
2. Iteratively solve $(K - \omega_n^2 M)\mathrm{u}_{n+1} = M\mathrm{u}_n$; the solution converges to the nearest eigenvector
3. At the end of the iteration, normalize the eigenvector by $|\mathrm{u}_n|_\infty$
4. and then evaluate $\omega_n^2 = \mathrm{u}_n \cdot K \cdot \mathrm{u}_n / \mathrm{u}_n \cdot M \cdot \mathrm{u}_n$



mode 1



mode 2



mode 3

Transposing Sauvan's method to elastodynamics – 1

[Sauvan et al. Physical Review Letters **110** 237401 (2013)]
Consider two different solutions of the elastodynamic equation ($\alpha = 1, 2$):

$$\mathrm{F}_\alpha + \nabla \cdot (c : \nabla \mathrm{u}_\alpha) = \frac{\partial}{\partial t}\left(\rho \frac{\partial \mathrm{u}_\alpha}{\partial t}\right) \tag{5}$$

Weak form of the equation for one solution with the test function as the other solution:

$$\int S_2 : c(\omega_1) : S_1 - \omega_1^2 \int \mathrm{u}_2 \cdot \rho(\omega_1)\mathrm{u}_1 = \int \mathrm{u}_2 \cdot \mathrm{F}_1 \tag{6}$$

and the same equation with indices 1 and 2 permuted. Their difference leads to

$$\int S_2 : [c(\omega_1) - c(\omega_2)] : S_1 - \int \mathrm{u}_2 \cdot [\omega_1^2 \rho(\omega_1) - \omega_2^2 \rho(\omega_2)]\mathrm{u}_1 = \int \mathrm{u}_2 \cdot \mathrm{F}_1 - \mathrm{u}_1 \cdot \mathrm{F}_2 \tag{7}$$

Transposing Sauvan's method to elastodynamics – 2

Take sol. 2 as QNM number n and sol. 1 as the forced elastodynamic solution at ω:

$$\int S_n : [c(\omega) - c(\omega_n)] : S - \int \mathrm{u}_n \cdot [\omega^2 \rho(\omega) - \omega_n^2 \rho(\omega_n)]\mathrm{u} = \int \mathrm{u}_n \cdot \mathrm{F}, \forall n \tag{8}$$

The QNMs constitute a basis for the solution (eigenfunction expansion theorem):

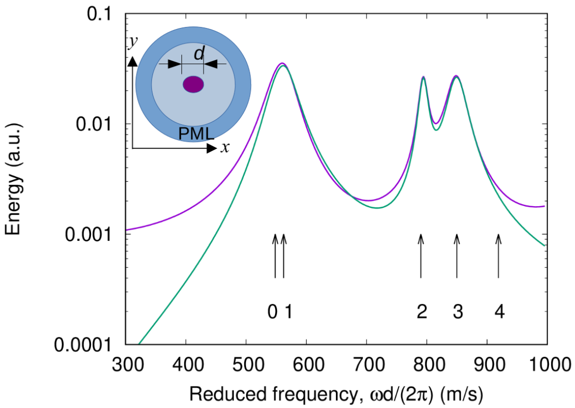
$$\mathrm{u}(\omega) = \sum_m \alpha_m(\omega)\mathrm{u}_m \tag{9}$$

$$\sum_m B_{nm}(\omega)\alpha_m(\omega) = \int \mathrm{u}_n \cdot \mathrm{F} = F_n, \forall n \tag{10}$$

$$B_{nm}(\omega) = \int S_n : [c(\omega) - c(\omega_n)] : S_m - \int \mathrm{u}_n \cdot [\omega^2 \rho(\omega) - \omega_n^2 \rho(\omega_n)]\mathrm{u}_m \tag{11}$$

If the QNMs are known, the $B_{nm}(\omega)$ coefficients are easily computed, and the $\alpha_m(\omega)$ are obtained by solving a linear problem as a function of frequency.

An elliptical nylon rod in water



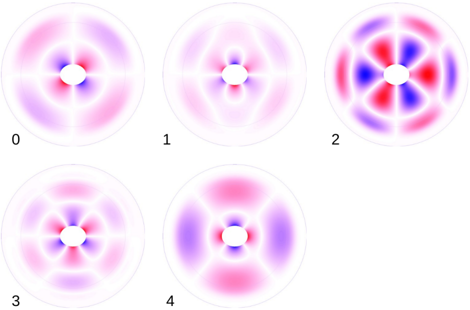


TABLE I. Characteristics for the QNMs of a cylindrical nylon rod immersed in water. The reduced frequency is $\omega d/(2\pi)$ with d the diameter of the rod.

Mode	0	1	2	3	4
Reduced frequency (m/s)	548	562	790	850	919
Q	12	48	24	30	12

Poling the response using QNMs

Sauvan's trick is to pole the previous equation by defining

$$A_{nm}(\omega) = \frac{1}{\omega - \omega_m} B_{nm}(\omega) \tag{12}$$

$$= \frac{1}{\omega - \omega_m}\left[\int S_n : [c(\omega) - c(\omega_n)] : S_m - \int \mathrm{u}_n \cdot [\omega^2 \rho(\omega) - \omega_n^2 \rho(\omega_n)]\mathrm{u}_m\right] \tag{13}$$

$A_{nm}(\omega_n) = 0$ if $m \neq n$ and

$$A_{nn}(\omega_n) = \int S_n : \frac{\partial c}{\partial \omega}(\omega_n) : S_n - \int \mathrm{u}_n \cdot \frac{\partial(\omega^2 \rho(\omega))}{\partial \omega}(\omega_n)\mathrm{u}_n \tag{14}$$

In the viscoelastic case (μ is the phonon viscosity tensor):

$$A_{nn}(\omega_n) = -2\omega_n \int \mathrm{u}_n \cdot \rho \mathrm{u}_n + \imath \int S_n : \mu : S_n \tag{15}$$

In the vicinity of each QNM:

$$\alpha_n(\omega) \approx \frac{1}{\omega - \omega_n} \frac{F_n}{A_{nn}(\omega_n)} + \Sigma_n(\omega) \tag{16}$$

Complex modal volume for QNMs

Considering some point in space r_0, the modal volume is

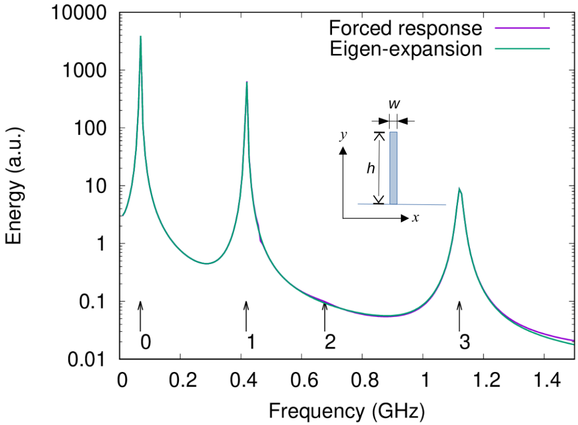
$$V_n = \frac{A_{nn}(\omega_n)}{2\omega_n[\rho(r_0)u_n^2(r_0)]} \tag{17}$$

$$r_0 = \underset{r}{\operatorname{argmax}}\,|\rho(r)u_n^2(r)| \tag{18}$$

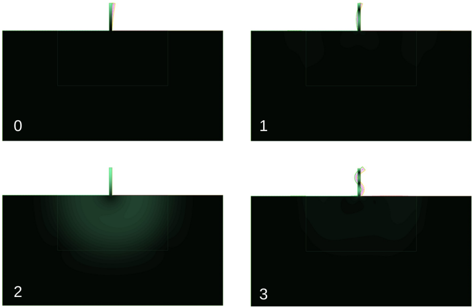
The modal volume is insensitive to multiplication by an arbitrary complex number. Indeed, QNMs are defined up to a complex multiplication constant only, as all eigenmodes. At resonance, $\omega \approx \Re\omega_n$ and the 'phononic Purcell effect' is

$$\mathrm{u}(\Re\omega_n) \approx -i\frac{1}{\omega_n\Re\omega_n[\rho(\mathrm{r}_0)u_n^2(\mathrm{r}_0)]}\frac{Q_n}{V_n}F_n\mathrm{u}_n. \tag{19}$$

A nanoscale nickel strip on fused silica ($F_x = 1$)

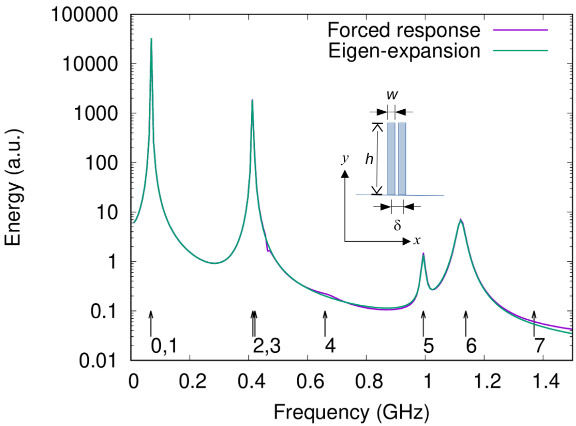


$w = 100$ nm, $h = 1000$ nm, 2D (strip) geometry

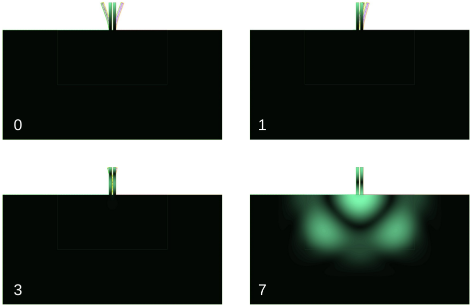


Mode	freq. (GHz)	Q	volume (μm^2)	polarization
0	0.0681	12600	0.0272	(0.997, 0.003, 0)
1	0.417	1000	0.0277	(0.979, 0.021, 0)
2	0.676	9	0.0923	(0, 0, 1)
3	1.12	60	0.0285	(0.959, 0.041, 0)

A nanoscale nickel tuning fork on fused silica ($F_x = 1$)



$w = 100$ nm, $h = 1000$ nm, $\delta = 50$ nm



Mode	freq. (GHz)	Q	volume (μm^2)	polarization
0	0.0674	240000	0.0536	$(0.997, 0.003, 0)$
1	0.0689	6700	0.0533	$(0.997, 0.003, 0)$
2	0.414	334	0.0569	$(0.979, 0.021, 0)$
3	0.421	4200	0.0524	$(0.972, 0.028, 0)$
4	0.659	3200	0.113	$(0, 0, 1)$
5	0.993	82	0.103	$(0.01, 0.99, 0)$
6	1.137	200	0.0365	$(0.957, 0.043, 0)$
7	1.369	10	0.474	$(0, 0, 1)$

Transposing Sauvan's method to acoustic waves – 1

The acoustic equation at frequency ω replacing the elastodynamic equation is

$$-\nabla \cdot (\rho^{-1} \nabla p) - \omega^2 B^{-1} p = \nabla \cdot (\rho^{-1} \mathrm{F}) = g \tag{20}$$

for pressure field $p(\mathrm{r})$ (a scalar field) and body force $\mathrm{F}(\mathrm{r})$. $B(\mathrm{r})$ is the elastic modulus and can be dispersive. The scalar source field $g(\mathrm{r})$ is introduced for convenience.

$$\int \nabla p_2 \rho_1^{-1} \nabla p_1 - \omega_1^2 \int p_2 B_1^{-1} p_1 = \int p_2 g_1 \tag{21}$$

with $\rho_1^{-1} = \rho^{-1}(\omega_1)$ and $B_1^{-1} = B^{-1}(\omega_1)$.

$$\int \nabla p_2 [\rho_1^{-1} - \rho_2^{-1}] \nabla p_1 \ - \int p_2 [\omega_1^2 B_1^{-1} - \omega_2^2 B_2^{-1}] p_1 \ = \int p_2 g_1 - p_1 g_2 . \tag{22}$$

Transposing Sauvan's method to acoustic waves – 2

Take solution 2 as QNM number n and solution 1 as the current solution p depending on ω,

$$\int \nabla p_n[\rho^{-1}(\omega) - \rho_n^{-1}]\nabla p - \int p_n[\omega^2 B^{-1}(\omega) - \omega_n^2 B_n^{-1}]p = \int p_n g, \forall n. \tag{23}$$

The QNMs constitute a basis for the solution (per the eigenfunction expansion theorem),

$$p(\omega) = \sum_m \beta_m(\omega) p_m. \tag{24}$$

$$\sum_m D_{nm}(\omega)\beta_m(\omega) = \int p_n g = g_n, \forall n \tag{25}$$

with

$$D_{nm}(\omega) = \int \nabla p_n[\rho^{-1}(\omega) - \rho_n^{-1}]\nabla p_m - \int p_n[\omega^2 B^{-1}(\omega) - \omega_n^2 B_n^{-1}]p_m. \tag{26}$$

If the QNMs are known, the $D_{nm}(\omega)$ coefficients are easily computed, and the $\beta_m(\omega)$ are obtained by solving a small linear problem as a function of frequency.

Transposing Sauvan's method to acousto-elastic resonances

$$\omega^2 \int_{\Omega_e} \mathrm{v} \cdot \rho_e \mathrm{u} - \int_{\Omega_e} S(\mathrm{v}) : c : S(\mathrm{u}) - \int_{\sigma_e} v_n p - \omega^{-2} \int_{\Omega_a} \nabla q \rho_a^{-1} \nabla p + \int_{\Omega_a} q B^{-1} p + \int_{\sigma_a} u_n q = \int_{\Omega_e} \mathrm{v} \cdot \mathrm{F} \quad (27)$$

$$B_{nm}(\omega) = \int_{\Omega_e} S_n : [c(\omega) - c(\omega_n)] : S_m - \int_{\Omega_e} \mathrm{u}_n \cdot [\omega^2 \rho(\omega) - \omega_n^2 \rho(\omega_n)] \mathrm{u}_m$$
$$+ \int_{\Omega_a} \nabla p_n [\omega^{-2} \rho^{-1}(\omega) - \omega_n^{-2} \rho_n^{-1}] \nabla p_m - \int_{\Omega_a} p_n [B^{-1}(\omega) - B_n^{-1}] p_m. \quad (28)$$

$$\mathrm{u}(\omega) = \sum_m \alpha_m(\omega) \mathrm{u}_m, \quad p(\omega) = \sum_m \alpha_m(\omega) p_m \quad (29)$$

Coefficients $\alpha_m(\omega)$ are obtained by solving

$$\sum_m B_{nm}(\omega) \alpha_m(\omega) = \int_{\Omega_e} \mathrm{u}_n \cdot \mathrm{F} = F_n, \forall n. \quad (30)$$

Conclusion and outlook

- Quasi-normal modes are the eigenmodes of resonant (open) structures
- Their eigenfrequencies can be obtained in the complex plane; the modal shape is obtained in the process
- Material dispersion and loss are accounted for
- Their modal volume is complex-valued!
- Only a small number of QNMs are required to 'predict' the frequency response for any excitation
- Theory provided for elastodynamics, acoustics, and acousto-elasticity

V. Laude and Y.-F. Wang, Phys. Rev. B 107, 144301 (2023)
https://doi.org/10.1103/PhysRevB.107.144301

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