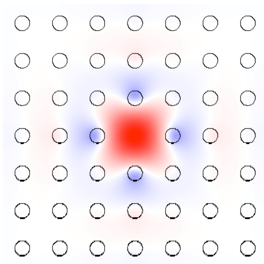
Microcavity Blues

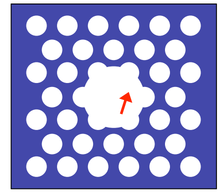


For cavities (*point defects*)
frequency-domain has its drawbacks:

- Best methods compute lowest-ω bands, but N^d supercells have N^d modes below the cavity mode — *expensive*
- Best methods are for Hermitian operators, but losses requires non-Hermitian

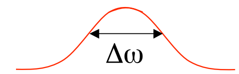
Time-Domain Eigensolvers

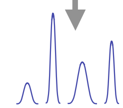
(finite-difference time-domain = FDTD)



Simulate Maxwell's equations on a discrete grid,
+ absorbing boundaries (leakage loss)

- Excite with broad-spectrum dipole (↑) source





Response is many sharp peaks, one peak per mode

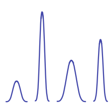
signal processing

complex ω_n

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

decay rate in time gives loss

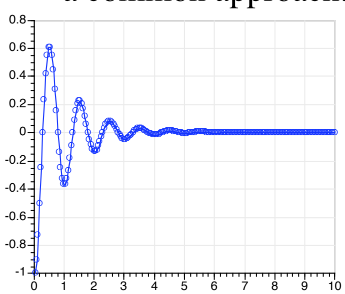
Signal Processing is Tricky



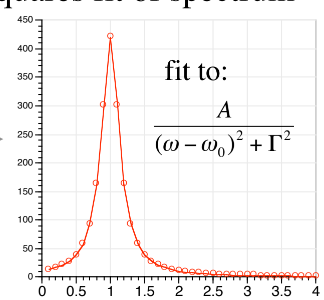
signal processing → complex ω_n

?

a common approach: least-squares fit of spectrum



FFT



fit to:

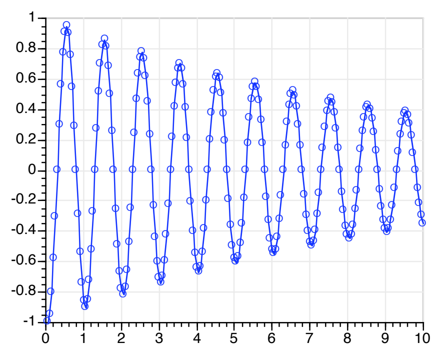
$$\frac{A}{(\omega-\omega_0)^2+\Gamma^2}$$

Decaying signal (*t*)

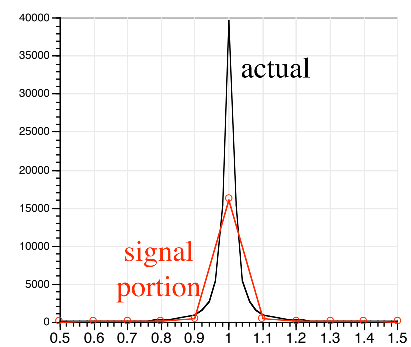
Lorentzian peak (ω)

Fits and Uncertainty

problem: have to run long enough to *completely* decay



Portion of decaying signal (*t*)



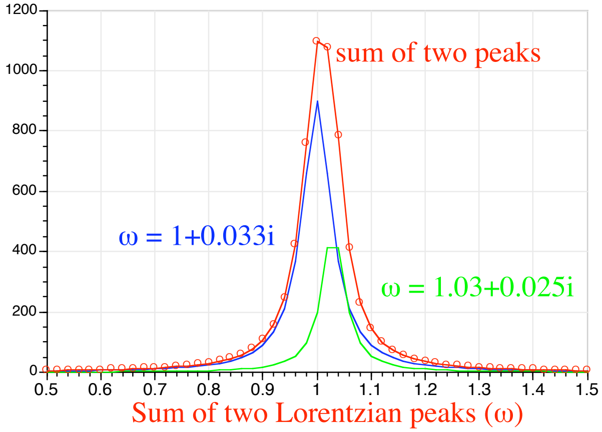
Unresolved Lorentzian peak (ω)

There is a better way, which gets complex ω to > 10 digits

Unreliability of Fitting Process

Resolving two overlapping peaks is near-impossible 6-parameter nonlinear fit

(too many local minima to converge reliably)



There is a better way, which gets complex ω for *both* peaks to > 10 digits

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Quantum-inspired signal processing (NMR spectroscopy):

Filter-Diagonalization Method (FDM)

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

Given time series y_n, write: $$y_n = y(n\Delta t) = \sum_k a_k e^{-i\omega_k n\Delta t}$$

…find *complex* amplitudes a_k & frequencies ω_k by a simple linear-algebra problem!

Idea: pretend $y(t)$ is autocorrelation of a quantum system:

$$\hat{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle \qquad \text{time-}\Delta t\text{ evolution-operator: } \hat{U} = e^{-i\hat{H}\Delta t/\hbar}$$

say: $$y_n = \langle\psi(0)|\psi(n\Delta t)\rangle = \langle\psi(0)|\hat{U}^n|\psi(0)\rangle$$

Filter-Diagonalization Method (FDM)

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

$$y_n = \langle\psi(0)|\psi(n\Delta t)\rangle = \langle\psi(0)|\hat{U}^n|\psi(0)\rangle \qquad \hat{U} = e^{-i\hat{H}\Delta t/\hbar}$$

We want to diagonalize U: eigenvalues of U are $e^{i\omega\Delta t}$

…expand U in basis of $|\psi(n\Delta t)>$:

$$U_{m,n} = \langle\psi(m\Delta t)|\hat{U}|\psi(n\Delta t)\rangle = \langle\psi(0)|\hat{U}^m\hat{U}\hat{U}^n|\psi(0)\rangle = y_{m+n+1}$$

U_{mn} given by y_n's — just diagonalize known matrix!

Filter-Diagonalization Summary

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

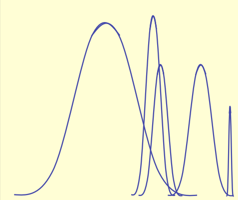
U_{mn} given by y_n's — just diagonalize known matrix!

A few omitted steps:

—Generalized eigenvalue problem (basis not orthogonal)

—Filter y_n's (Fourier transform):

small bandwidth = smaller matrix (less singular)



- resolves many peaks at once
- # peaks not known *a priori*
- resolve overlapping peaks
- resolution >> Fourier uncertainty