Microcavity Blues

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

- Best methods compute lowest-$\omega$ bands, but $N^d$ supercells have $N^d$ modes below the cavity mode — expensive
- Best methods are for Hermitian operators, but losses require 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 ($\dagger$) source

Response is many sharp peaks, one peak per mode

 decay rate in time gives loss

There is a better way, which gets complex $\omega$ to $> 10$ digits

Signal Processing is Tricky

a common approach: least-squares fit of spectrum

Decaying signal ($t$) Lorentzian peak ($\omega$)

Fits and Uncertainty

problem: have to run long enough to completely decay

Portion of decaying signal ($t$) Unresolved Lorentzian peak ($\omega$)

There is a better way, which gets complex $\omega$ 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)

Filter-Diagonalization Method (FDM)

Quantum-inspired signal processing (NMR spectroscopy):

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Quantum-inspired signal processing (NMR spectroscopy):

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 $\omega_k$ by a simple linear-algebra problem!

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

$$\hat{H}|\psi\rangle = \frac{i\hbar}{\hbar} \frac{\partial}{\partial t} |\psi\rangle$$

time-$\Delta t$ evolution-operator: $\hat{U} = e^{-i\hat{H}/\hbar}$

say:

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

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Filter-Diagonalization Summary

$U_{mn}$ 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