Computational Nanophotonics: Cavities and Resonant Devices

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Resonance

an oscillating mode trapped for a long time in some volume
(of light, sound, …)

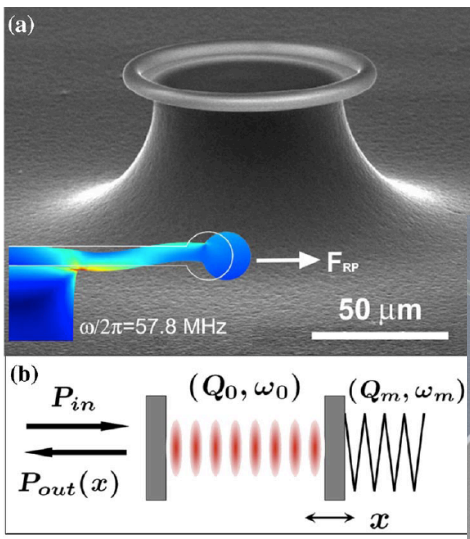
lifetime $\tau >> 2\pi/\omega_0$

frequency ω_0

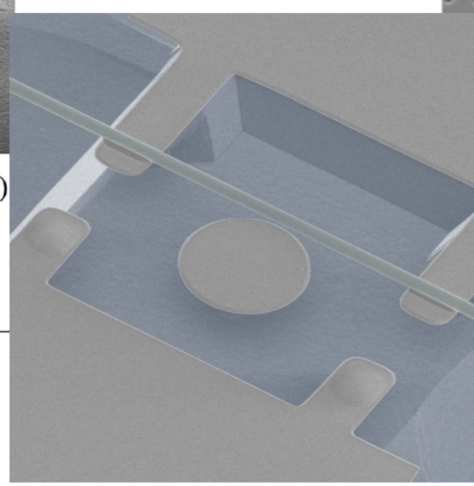
quality factor $Q = \omega_0\tau/2$

energy ~ $e^{-\omega_0 t/Q}$

modal volume V

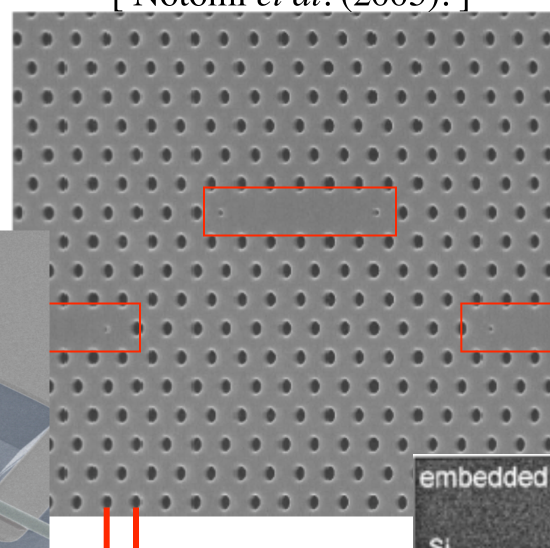


[Schliesser et al., *PRL* **97**, 243905 (2006)]



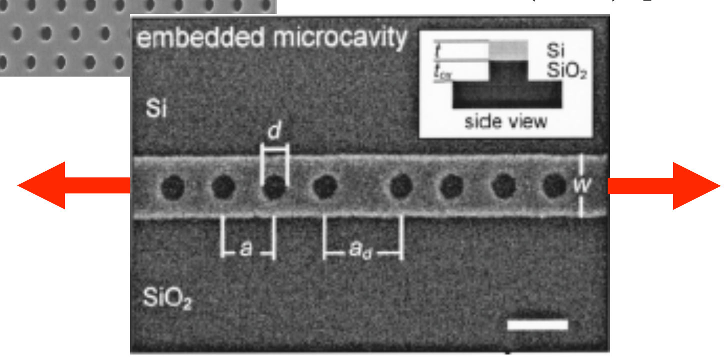
[Eichenfield et al. *Nature Photonics* **1**, 416 (2007)]

[Notomi *et al*. (2005).]



420 nm

[C.-W. Wong, *APL* **84**, 1242 (2004).]



Why Resonance?

an oscillating mode trapped for a long time in some volume

- long time = narrow bandwidth … filters (WDM, etc.)
  — $1/Q$ = fractional bandwidth

- resonant processes allow one to "impedance match" hard-to-couple inputs/outputs

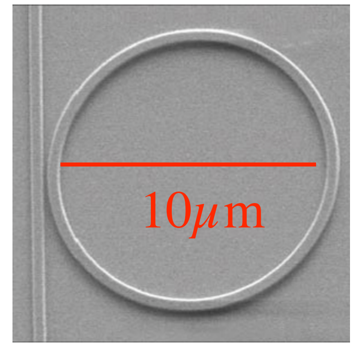
- long time, small V … enhanced wave/matter interaction
  — lasers, nonlinear optics, opto-mechanical coupling, sensors, LEDs, thermal sources, …

How Resonance?

need mechanism to trap light for long time

[llnl.gov]

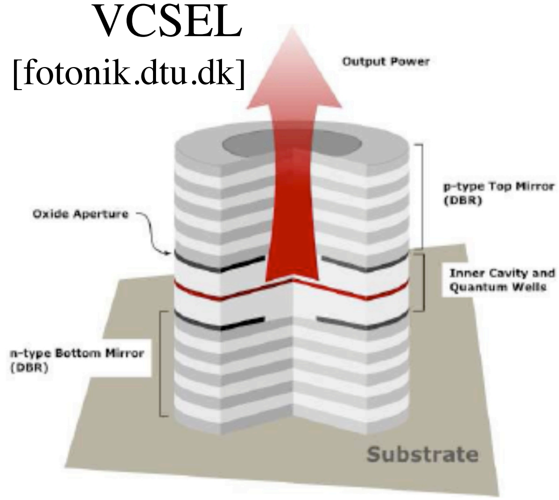
metallic cavities:
good for microwave,
dissipative for infrared

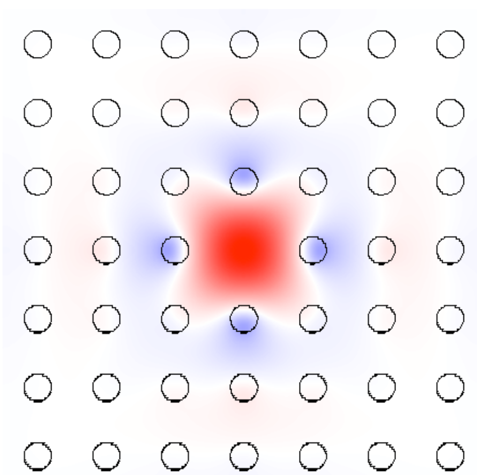


[Xu & Lipson (2005)]

ring/disc/sphere resonators:
a waveguide bent in circle,
bending loss ~ exp(–radius)

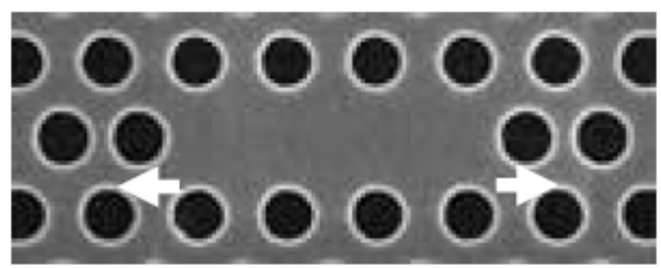
VCSEL
[fotonik.dtu.dk]





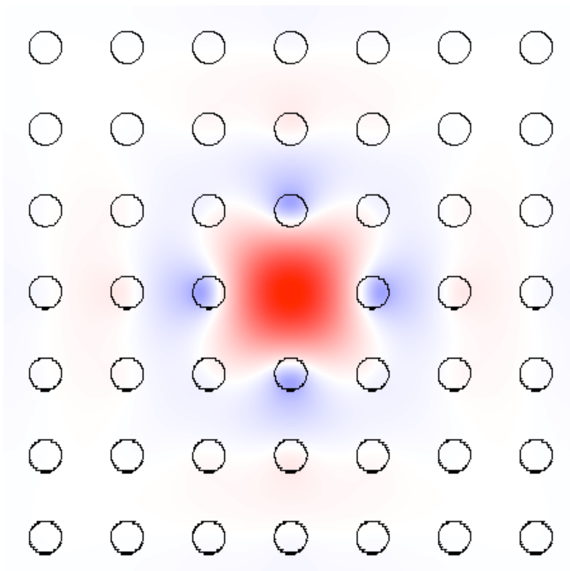
photonic bandgaps
(complete or partial
+ index-guiding)

[Akahane, *Nature* **425**, 944 (2003)]



(planar Si slab)

Microcavity Blues



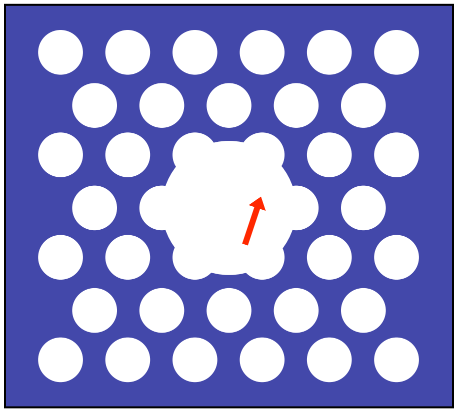
For cavities (*point defects*)
frequency-domain has its drawbacks:

- Best methods compute lowest-ω eigenvals,
  but N^d supercells have N^d modes
  below the cavity mode — *expensive*

- Best methods are for Hermitian operators,
  but losses requires non-Hermitian

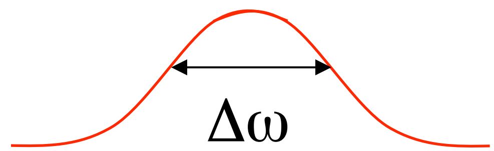
Time-Domain Eigensolvers

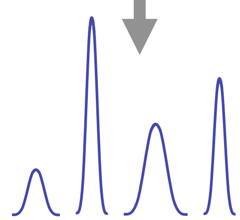
(finite-difference time-domain = FDTD)



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

tricky signal processing

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

complex ω_n

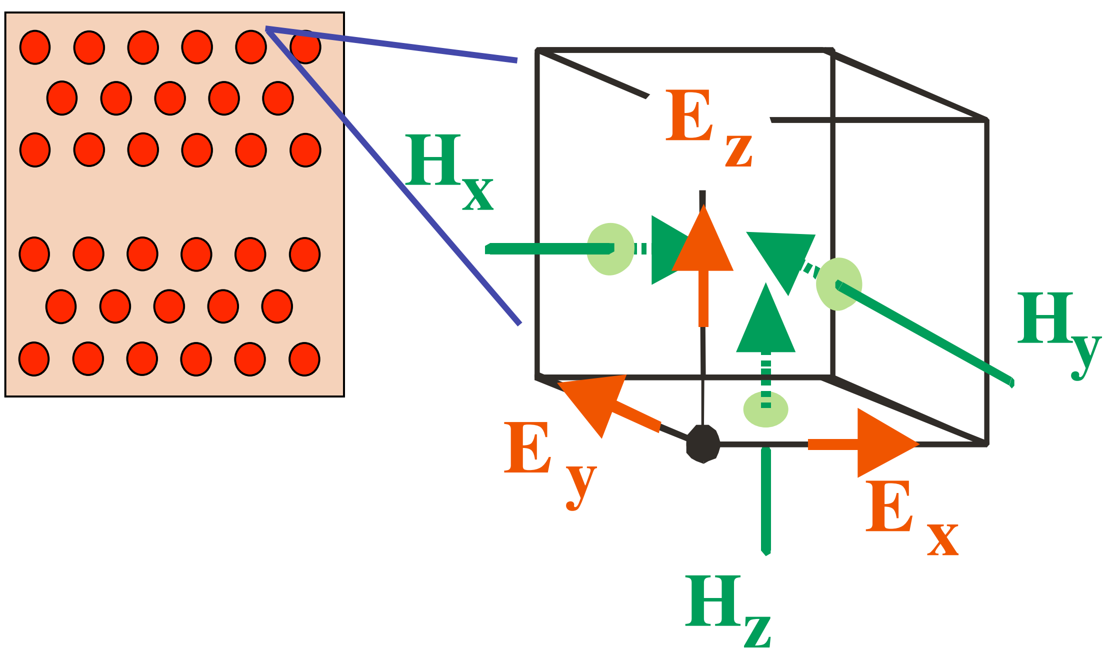
decay rate in time gives loss

FDTD: finite difference time domain

Finite-difference-time-domain (FDTD) is a method to model Maxwell's equations on a **discrete time** & **space grid** using finite centered differences

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\mathbf{D} = \varepsilon \mathbf{E} \qquad \mathbf{B} = \mu \mathbf{H}$$



K.S. Yee 1966

A. Taflove & S.C. Hagness 2005

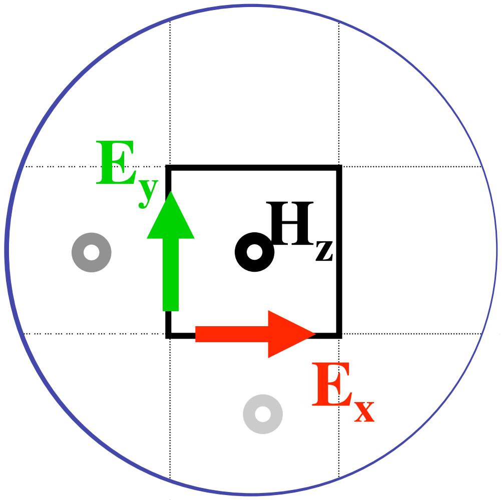
FDTD: Yee leapfrog algorithm

2d example:

1) **at time t: Update D fields everywhere using spatial derivatives of H, then find $E=\varepsilon^{-1}D$ (ε constant)**

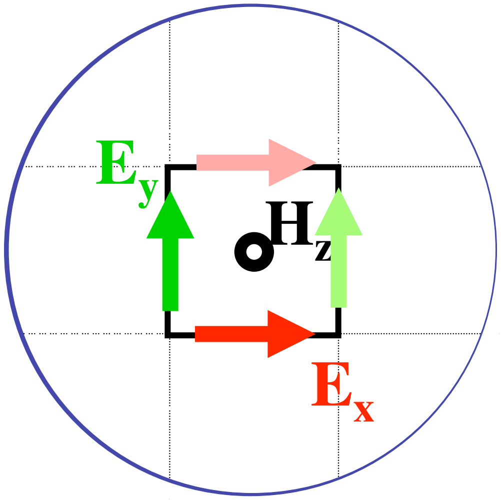
$$E_x \mathrel{+}= \frac{\Delta t}{\varepsilon\ \Delta y}\left(H_z^{j+0.5} - H_z^{j-0.5} \right)$$

$$E_y \mathrel{-}= \frac{\Delta t}{\varepsilon\ \Delta x}\left(H_z^{i+0.5} - H_z^{i-0.5} \right)$$



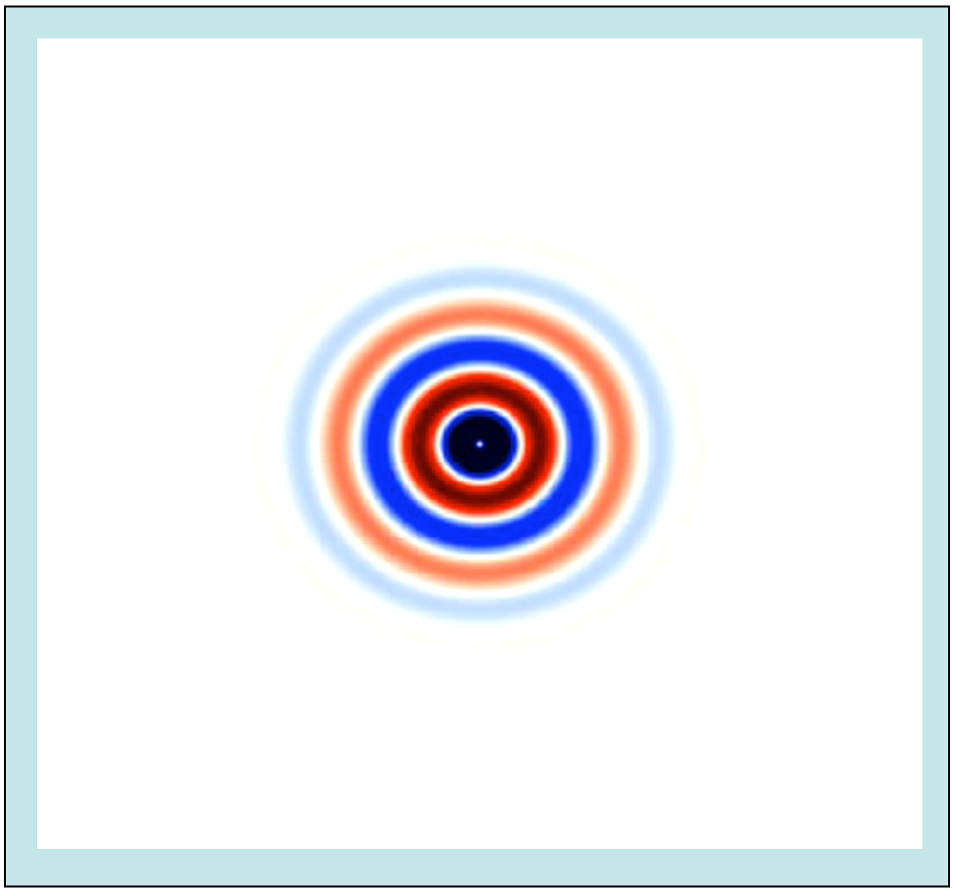
2) **at time t+0.5: Update H fields everywhere using spatial derivatives of E (μ constant)**

$$H_z \mathrel{+}= \frac{\Delta t}{\mu}\left(\frac{E_x^{j+1} - E_x^{j}}{\Delta y} + \frac{E_y^{i} - E_y^{i+1}}{\Delta x} \right)$$



Why Absorbers?

Finite-difference/finite-element volume discretizations need to artificially truncate space for a computer simulation.



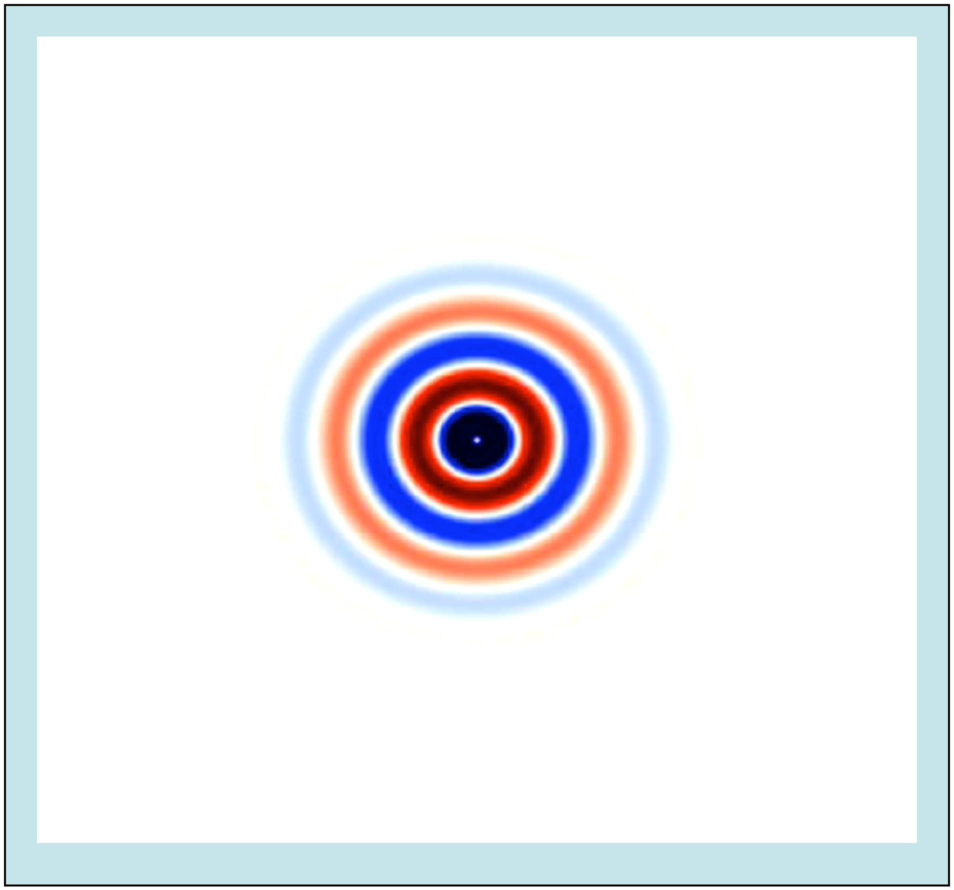
In a wave equation, a hard-wall truncation gives reflection artifacts.

An old goal: "absorbing boundary condition" (ABC) that absorbs outgoing waves.

Problem: good ABCs are hard to find in > 1d.

Perfectly Matched Layers (PMLs)

Bérenger, 1994: design an *artificial* absorbing layer
that is analytically reflectionless



Works *remarkably well*.

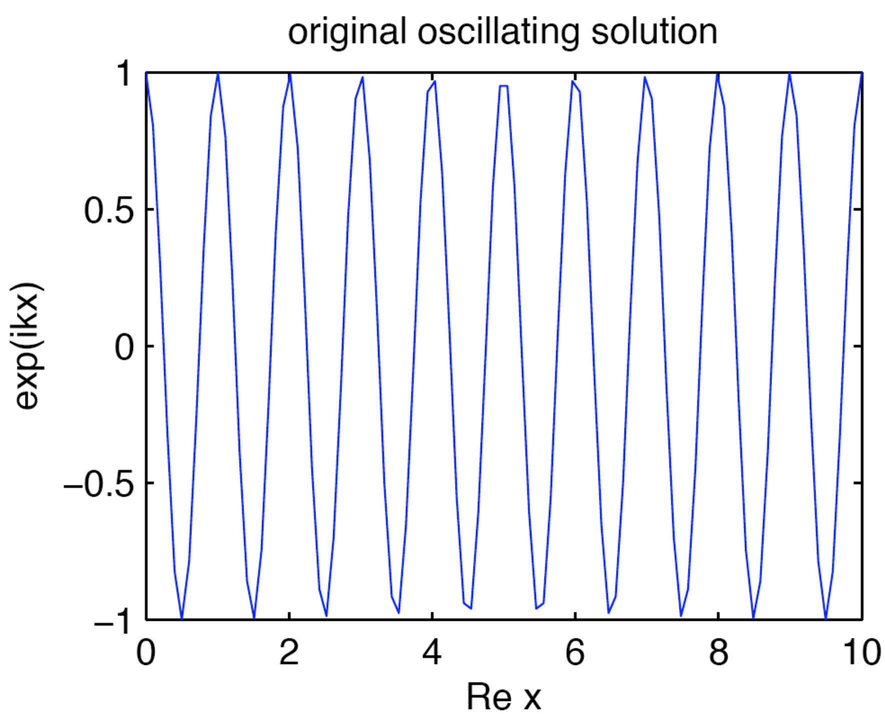
Now ubiquitous in FD/FEM wave-equation solvers.

Several derivations, cleanest & most general via "complex coordinate stretching"
[Chew & Weedon (1994)]

PML Starting point: propagating wave

- Say we want to absorb wave traveling in $+x$ direction in an x-invariant medium at a frequency $\omega > 0$.

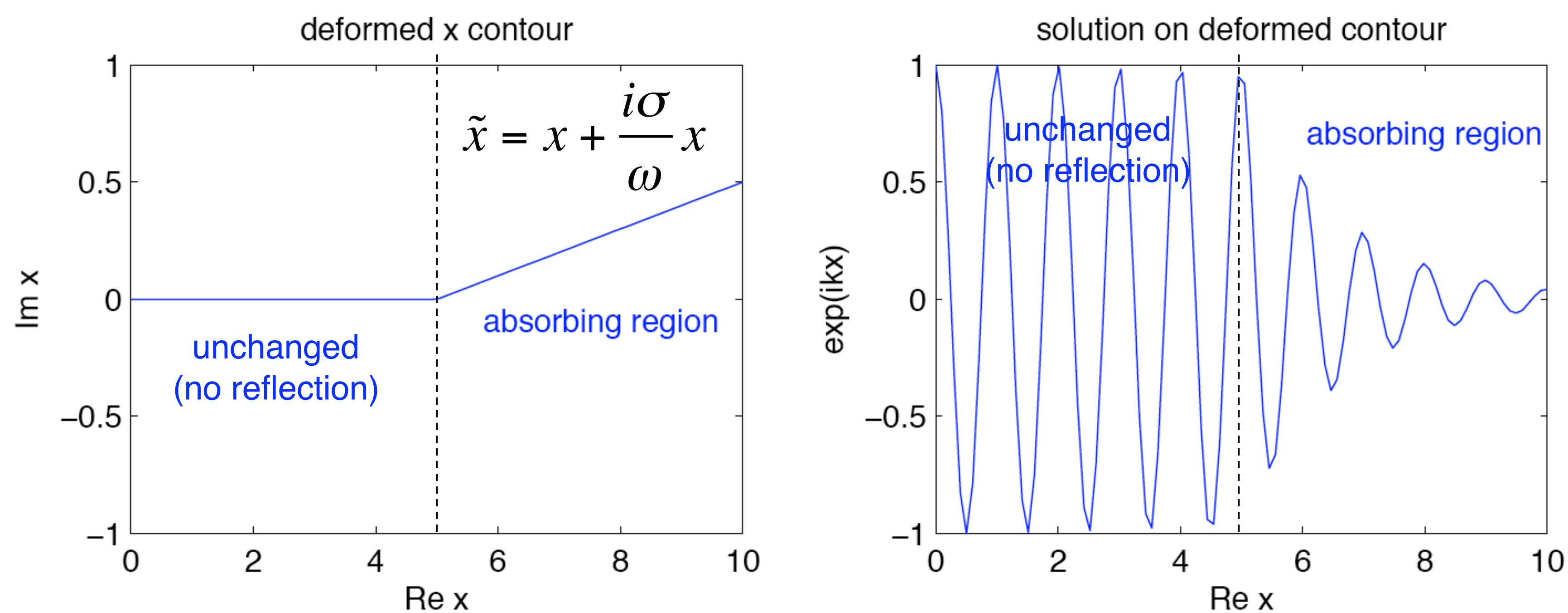
$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \qquad (usually, k > 0)$$



(only x in wave equation is via $\partial / \partial x$ terms.)

PML step 1: Analytically continue

Fields (& wave equation terms) are *analytic* in x,
so we can evaluate at complex x & still solve same equations



$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \to f(y,z)e^{i(kx-\omega t)-\frac{k}{\omega}\sigma x}$$

PML step 2: Coordinate transformation

Weird to solve equations for complex coordinates $\tilde{x}$,
so do coordinate transformation back to real x.

$$\tilde{x}(x) = x + \int^{x} \frac{i\sigma(x')}{\omega} dx'$$

(allow x-dependent PML strength σ)

$$\frac{\partial}{\partial x} \xrightarrow{①} \frac{\partial}{\partial \tilde{x}} \xrightarrow{②} \left[\frac{1}{1 + \frac{i\sigma(x)}{\omega}} \right] \frac{\partial}{\partial x}$$

$$\text{fields} \sim f(y,z) e^{i(kx-\omega t)} \rightarrow f(y,z) e^{i(kx-\omega t) - \frac{k}{\omega}\int^{x} \sigma(x')\,dx'}$$

nondispersive materials: $k/\omega \sim$ constant
⇒ decay rate independent of ω

PML Step 3: Effective materials

In Maxwell's equations, $\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E} + \mathbf{J}$,
coordinate transformations are *equivalent* to transformed *materials*
(Ward & Pendry, 1996: "transformational optics")

$$\{\varepsilon, \mu\} \to \frac{J\{\varepsilon, \mu\}J^T}{\det J}$$

x PML Jacobian

$$J = \begin{pmatrix} (1 + i\sigma/\omega)^{-1} & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$\left(\frac{\partial x}{\partial \tilde{x}}\right)$$

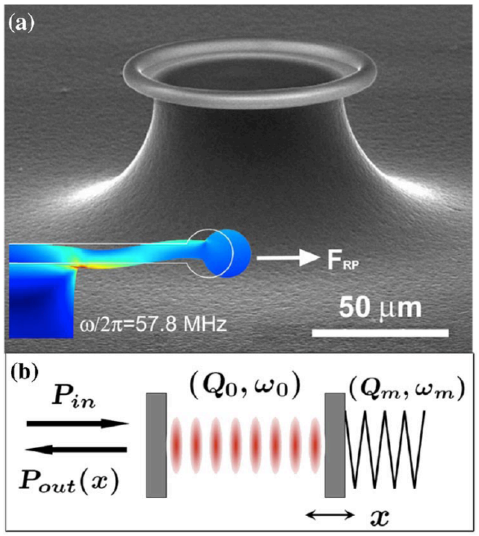
for isotropic starting materials:

$$\{\varepsilon, \mu\} \to \{\varepsilon, \mu\}\begin{pmatrix} (1 + i\sigma/\omega)^{-1} & & \\ & 1 + i\sigma/\omega & \\ & & 1 + i\sigma/\omega \end{pmatrix}$$

effective *conductivity*

PML = effective anisotropic "absorbing" ε, μ

Understanding Resonant Systems



[Schliesser et al., *PRL* **97**, 243905 (2006)]

- Option 1: Simulate the whole thing exactly
  - — many powerful numerical tools
  - — limited insight into a single system
  - — can be difficult, especially for weak effects (nonlinearities, etc.)

- Option 2: Solve each component separately, couple with explicit perturbative method (one kind of "coupled-mode" theory)

- Option 3: abstract the geometry into its most generic form
  …write down the *most general* possible equations
  …constrain by fundamental laws (conservation of energy)
  …solve for universal behaviors of a whole class of devices
  … characterized via specific parameters from option 2

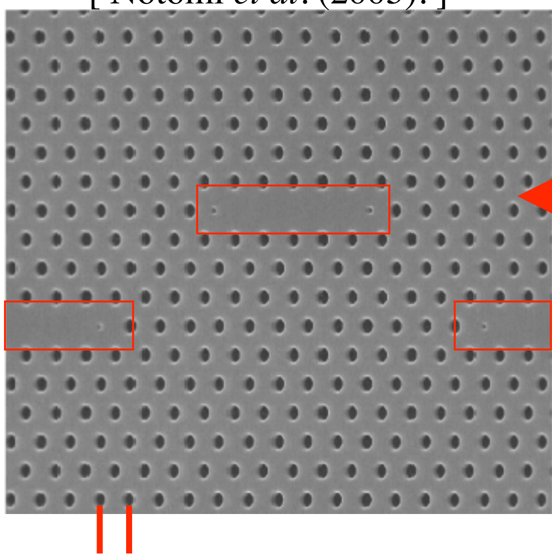
"Temporal coupled-mode theory"

- Generic form developed by Haus, Louisell, & others in 1960s & early 1970s
  - Haus, *Waves & Fields in Optoelectronics* (1984)
  - Reviewed in our *Photonic Crystals: Molding the Flow of Light*, 2nd ed., ab-initio.mit.edu/book
- Equations are generic ⇒ reappear in many forms in many systems, rederived in many ways (e.g. Breit–Wigner scattering theory)
  - full generality is not always apparent

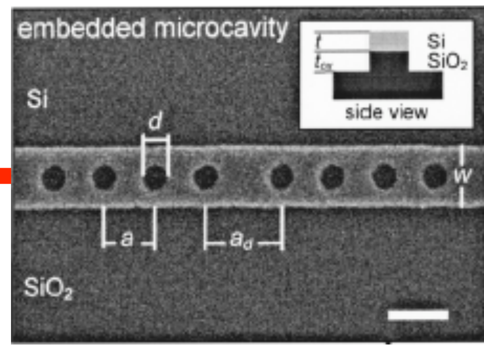
(modern name coined by S. Fan @ Stanford)

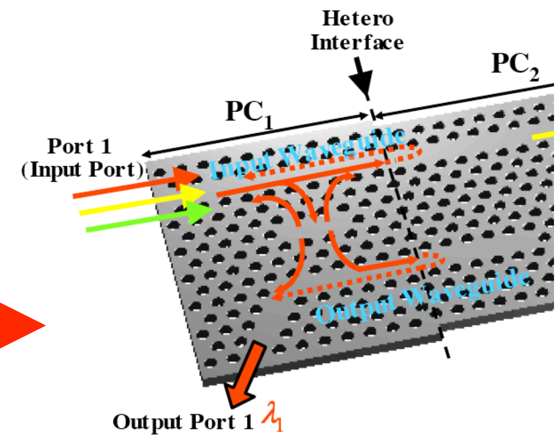
TCMT example: a linear filter

[Notomi *et al*. (2005).]

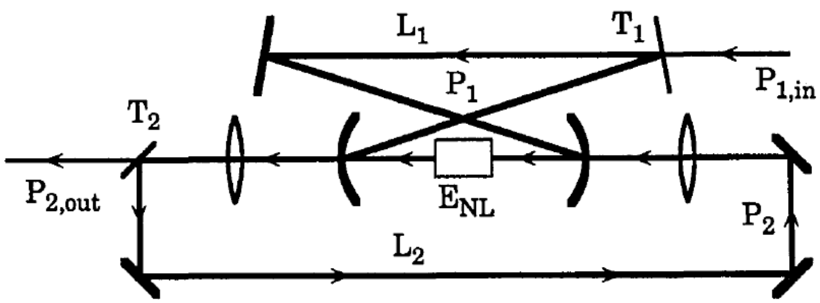


[C.-W. Wong,
APL **84**, 1242 (2004).]





[Takano *et al*. (2006)]

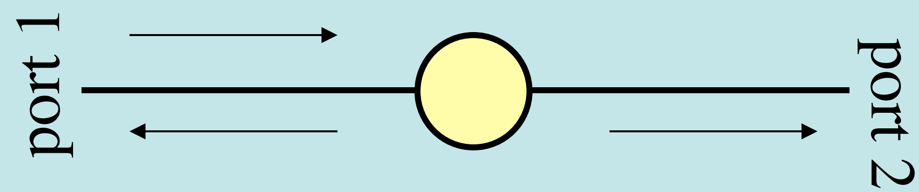


[Ou & Kimble (1993)]

= *abstractly:*

two single-mode i/o ports

+ one resonance

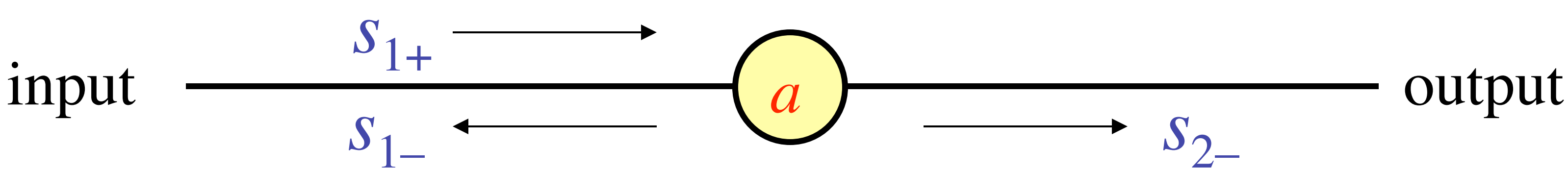


resonant cavity

frequency ω_0, lifetime τ

Temporal Coupled-Mode Theory

for a linear filter



resonant cavity
frequency ω_0, lifetime τ

$|s|^2$ = power

$|a|^2$ = energy

$$\frac{da}{dt} = -i\omega_0 a - \frac{2}{\tau}a + \sqrt{\frac{2}{\tau}}s_{1+}$$

$$s_{1-} = -s_{1+} + \sqrt{\frac{2}{\tau}}a, \quad s_{2-} = \sqrt{\frac{2}{\tau}}a$$

assumes only:

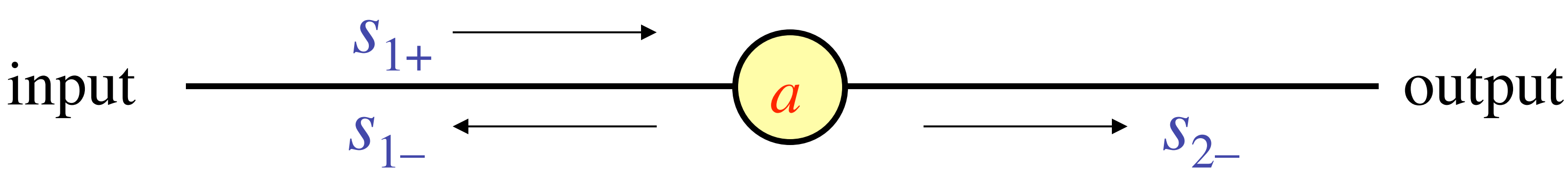
- exponential decay (strong confinement)

can be relaxed:

- linearity
- conservation of energy
- time-reversal symmetry

Temporal Coupled-Mode Theory

for a linear filter

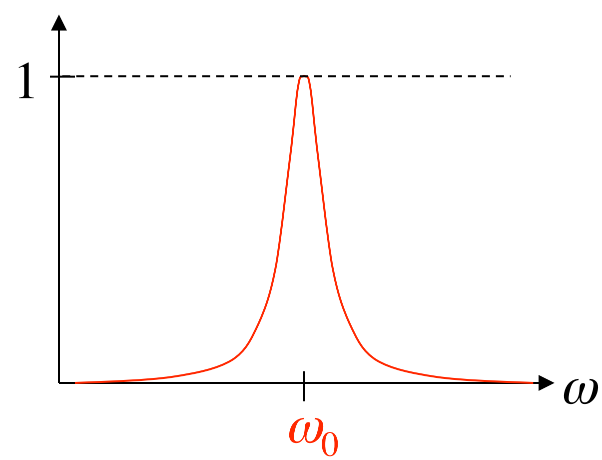


resonant cavity
frequency ω_0, lifetime τ

$|s|^2$ = flux

$|a|^2$ = energy

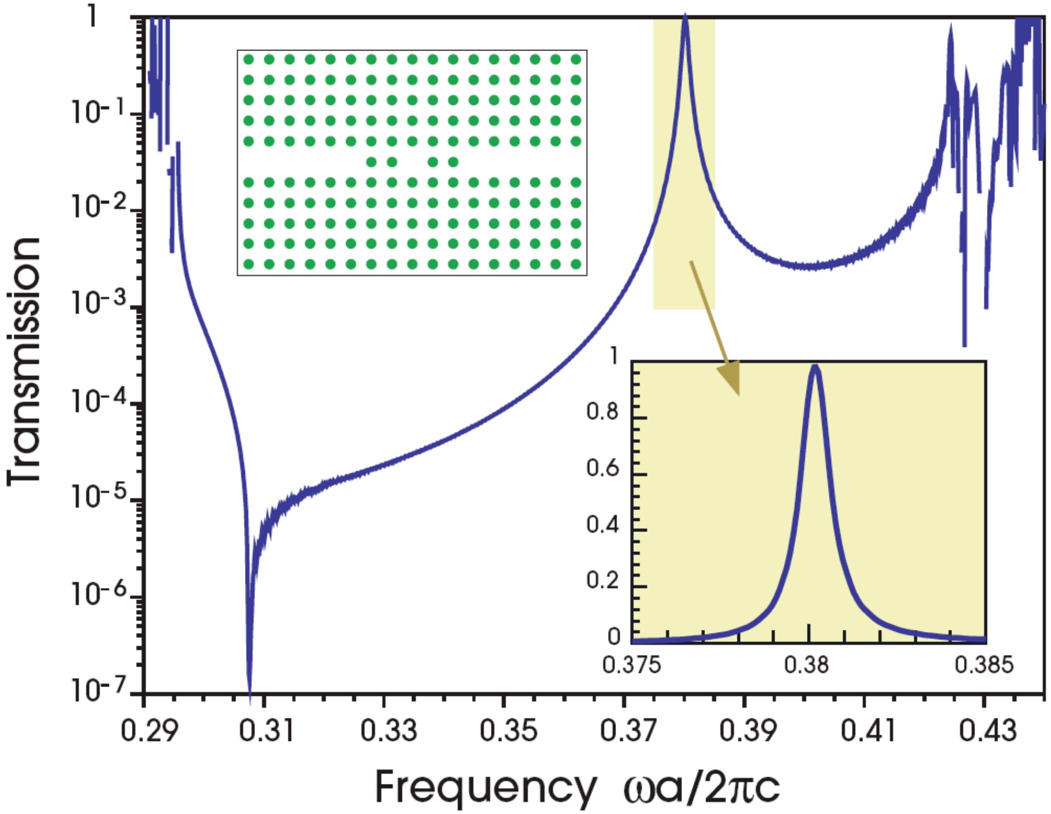
transmission T
$= | s_{2-} |^2 / | s_{1+} |^2$



T = Lorentzian filter

$$= \frac{\frac{4}{\tau^2}}{(\omega - \omega_0)^2 + \frac{4}{\tau^2}}$$

Resonant Filter Example

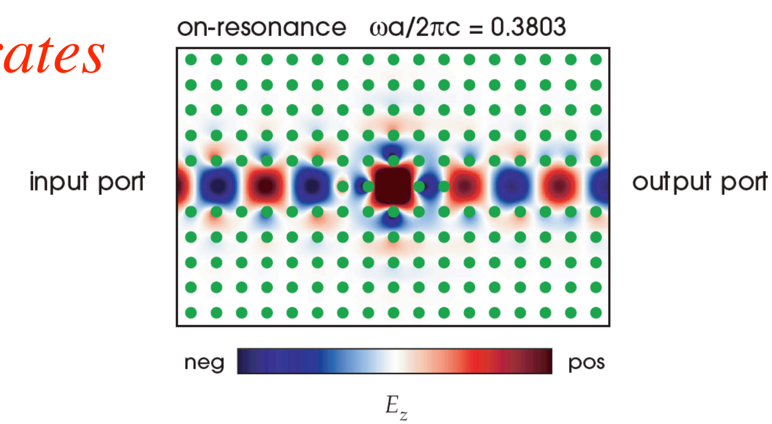


Lorentzian peak, as predicted.

An apparent miracle:

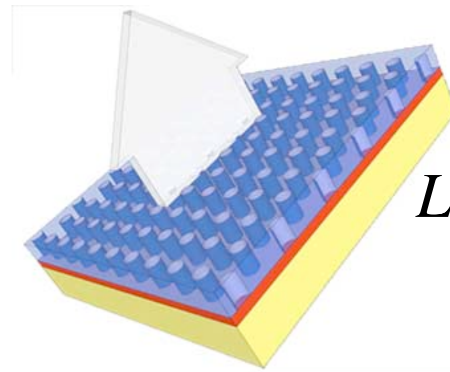
~ 100% transmission
at the resonant frequency

cavity decays to input/output with *equal rates*
⇒ At resonance, reflected wave
destructively interferes
with backwards-decay from cavity
& the two *exactly cancel*.

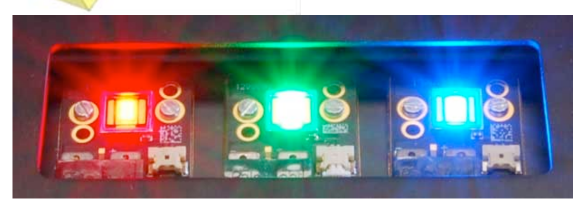


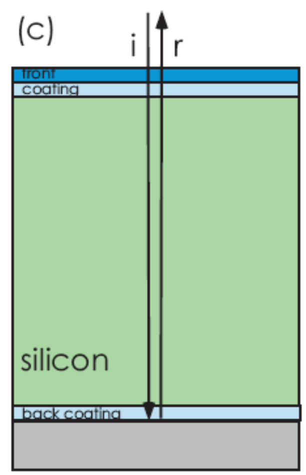
Some interesting resonant transmission processes

Wireless resonant power transfer
[M. Soljacic, MIT (2007)]
witricity.com



Resonant
LED emission
luminus.com

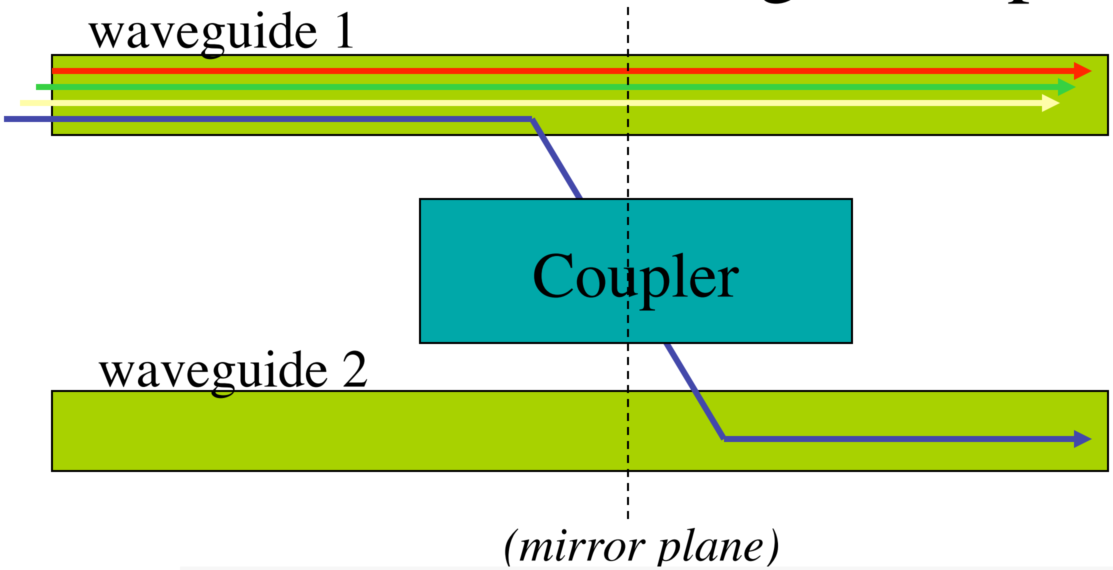




(narrow-band) resonant absorption in a thin-film photovoltaic

[e.g. Ghebrebrhan (2009)]

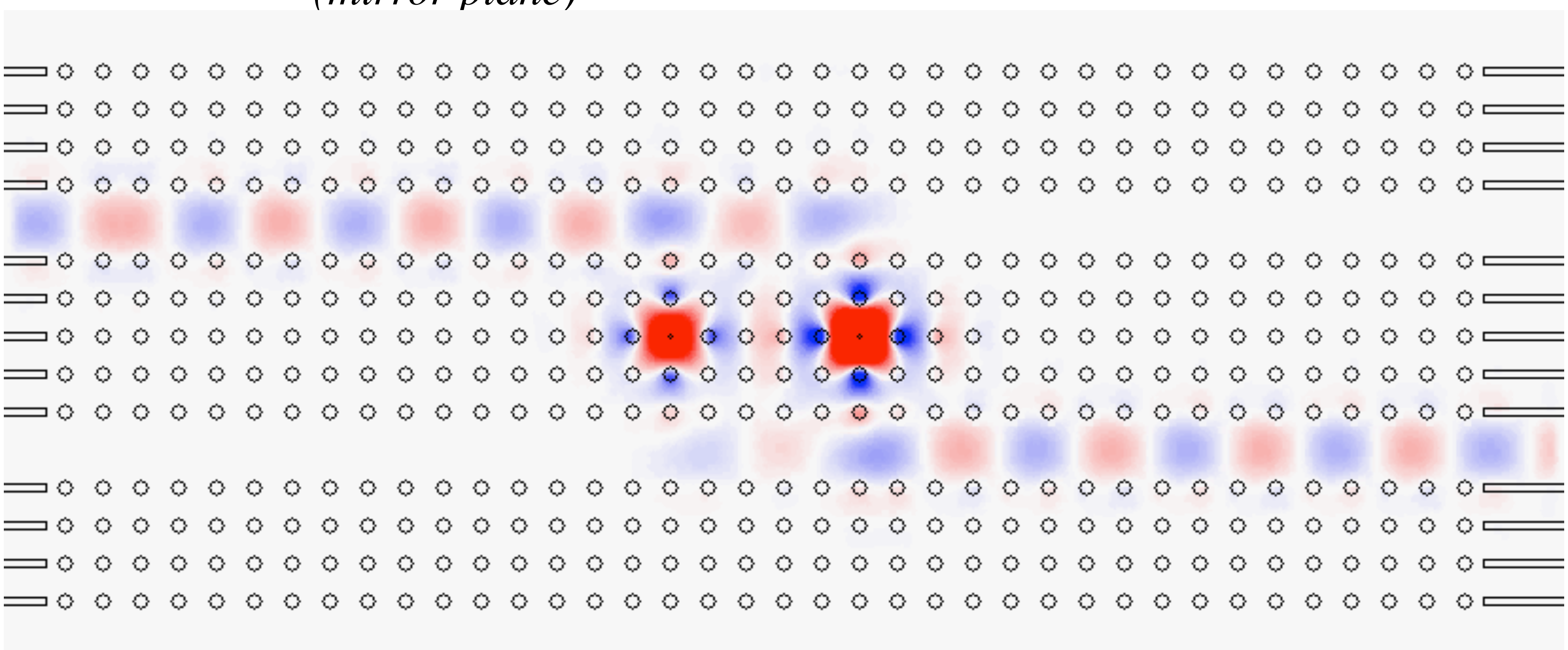
Another interesting example: Channel-Drop Filters



Perfect channel-dropping if:

Two resonant modes with:

- even and odd symmetry
- equal frequency (degenerate)
- equal decay rates



[S. Fan *et al*., *Phys. Rev. Lett*. **80**, 960 (1998)]

Dimensionless Losses: *Q*

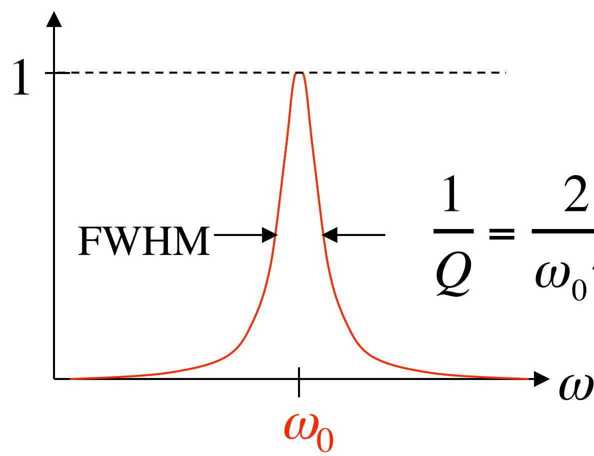
$$Q = \omega_0 \tau / 2$$

quality factor Q = # optical periods for energy to decay by exp(–2π)

energy ~ $\exp(-\omega_0 t/Q) = \exp(-2t/\tau)$

in frequency domain: $1/Q$ = bandwidth

from temporal coupled-mode theory:



$$\frac{1}{Q} = \frac{2}{\omega_0 \tau}$$

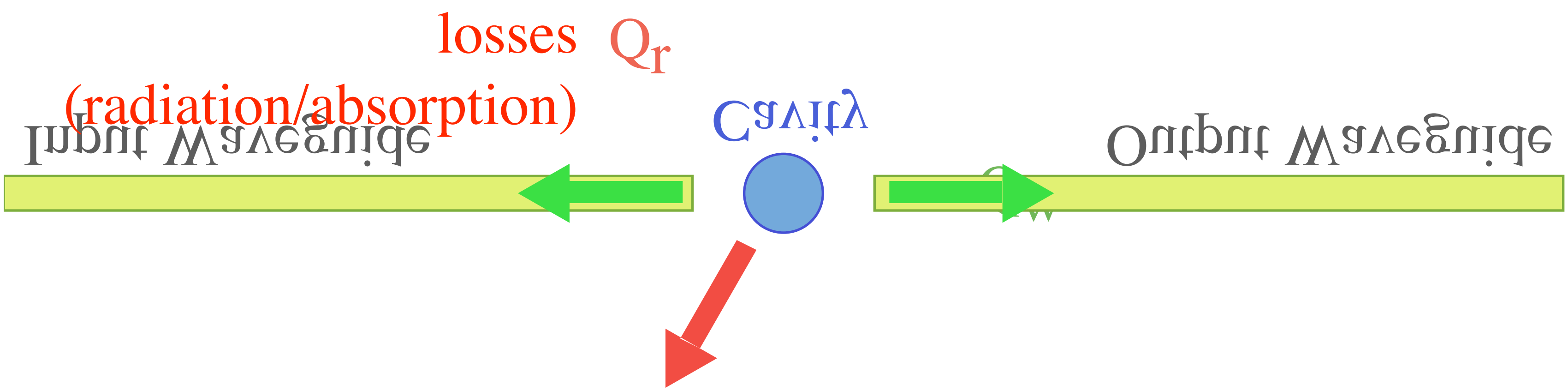
…quality factor Q

T = Lorentzian filter

$$= \frac{\frac{4}{\tau^2}}{(\omega - \omega_0)^2 + \frac{4}{\tau^2}}$$

More than one *Q*…

A simple model device (filters, bends, …):



$$\frac{1}{Q} = \frac{1}{Q_r} + \frac{1}{Q_w}$$

Q = lifetime/period
= frequency/bandwidth

We want: $Q_r >> Q_w$

TCMT ⇒

1 – transmission ~ $2Q / Q_r$

***worst case*:** high-Q (narrow-band) cavities

Nonlinearities + Microcavities?

weak effects — very intense fields

$\Delta n < 1\%$ — & sensitive to small changes

A simple idea:

for the same input power, nonlinear effects are stronger in a microcavity

That's not all!

nonlinearities + microcavities

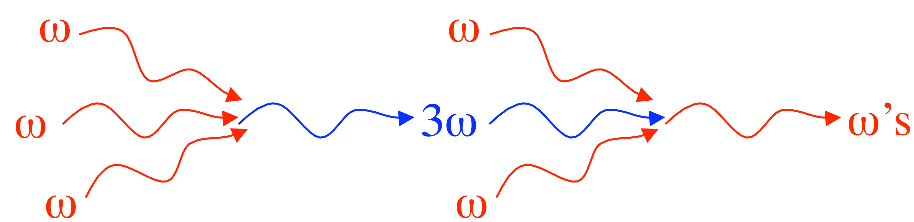
= *qualitatively* new phenomena

Nonlinear Optics

Kerr nonlinearities $\chi^{(3)}$: *(polarization ~ E^3)*

- Self-Phase Modulation (SPM)
  = change in refractive index(ω) ~ $|\mathbf{E}(\omega)|^2$
- Cross-Phase Modulation (XPM)
  = change in refractive index(ω) ~ $|\mathbf{E}(\omega_2)|^2$

- Third-Harmonic Generation (THG) & down-conversion (FWM)
  = $\omega \rightarrow 3\omega$, and back
- etc…



Second-order nonlinearities $\chi^{(2)}$: *(polarization ~ E^2)*

- Second-Harmonic Generation (SHG) & down-conversion
  = $\omega \rightarrow 2\omega$, and back
- Difference-Frequency Generation (DFG) = $\omega_1, \omega_2 \rightarrow \omega_1 - \omega_2$
- etc…

Nonlinearities + Microcavities?

weak effects | very intense fields
$\Delta n < 1\%$ | & sensitive to small changes

A simple idea:

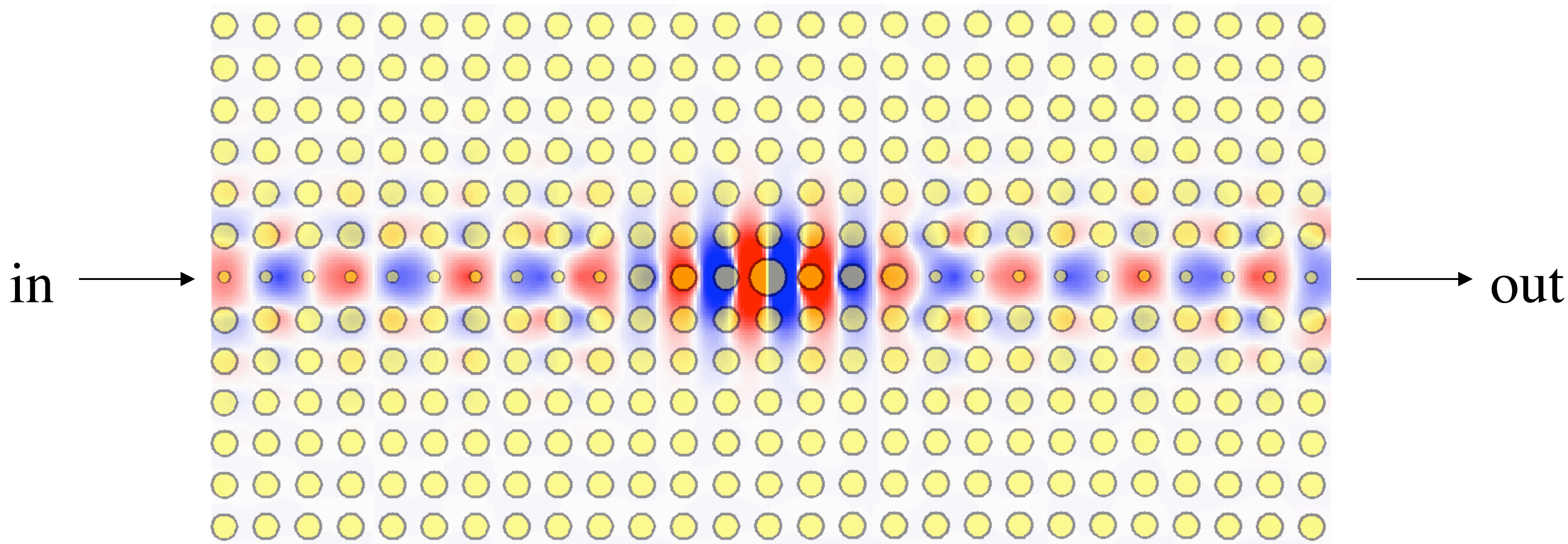
for the same input power, nonlinear effects are stronger in a microcavity

That's not all!

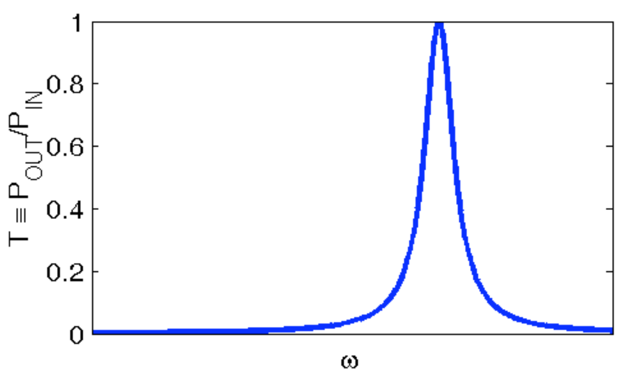
nonlinearities + microcavities
= *qualitatively* new phenomena

let's start with a well-known example from 1970's…

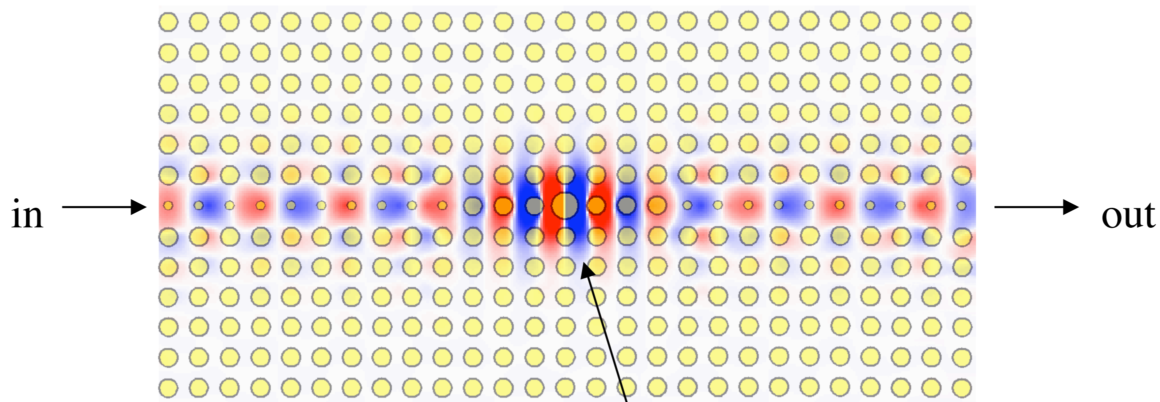
A Simple Linear Filter



Linear response:
Lorenzian Transmisson

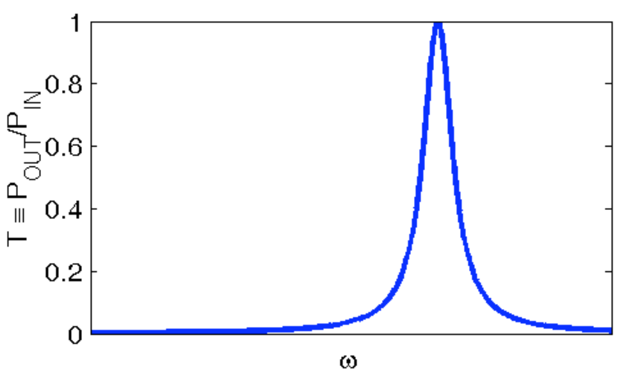


Filter + Kerr Nonlinearity?



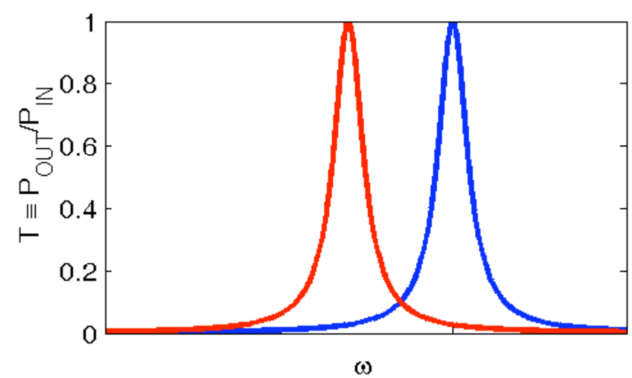
Kerr nonlinearity:
$\Delta n \sim |\mathbf{E}|^2$

Linear response:
Lorenzian Transmisson



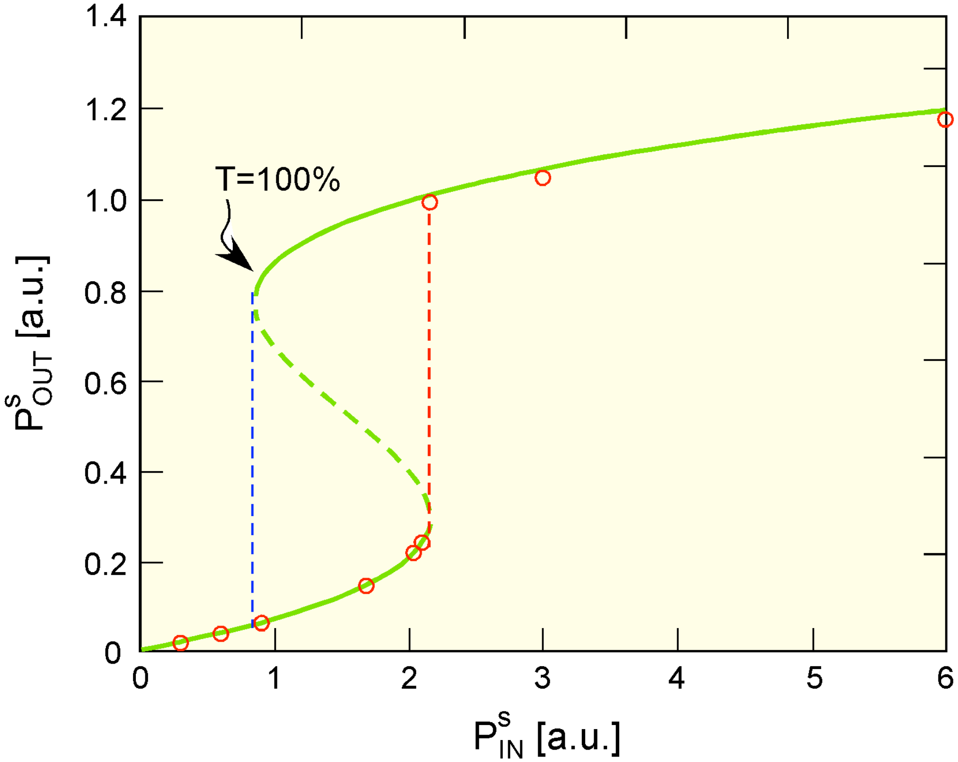
+ nonlinear
index shift
= ω shift

shifted peak?

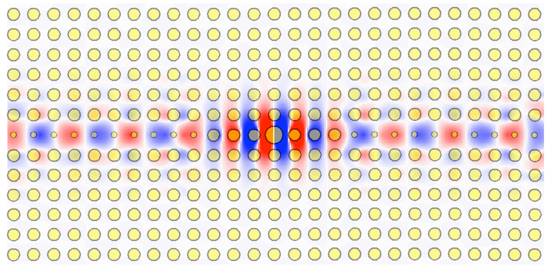


Optical Bistability

[Felber and Marburger., *Appl. Phys. Lett.* **28**, 731 (1978).]



Logic gates, switching, rectifiers, amplifiers, isolators, …



[Soljacic *et al.*, *PRE Rapid. Comm.* **66**, 055601 (2002).]

Bistable (hysteresis) response

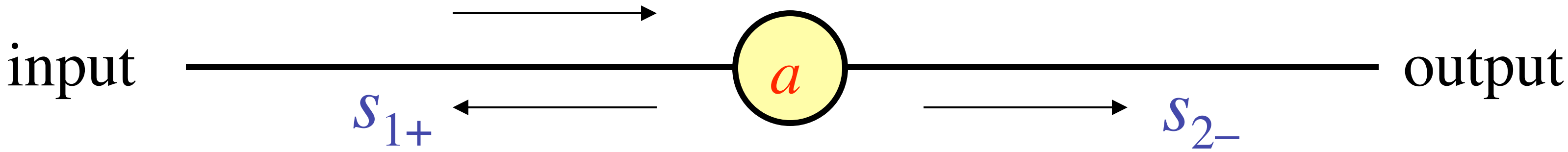
(& even multistable for multimode cavity)

Power threshold ~ V/Q^2

(in cavity with V ~ $(\lambda/2)^3$, for Si and telecom bandwidth power ~ mW)

TCMT for Bistability

[Soljacic *et al*., *PRE Rapid*. *Comm*. **66**, 055601 (2002).]



resonant cavity
frequency ω_0, lifetime τ,
SPM coefficient $\alpha \sim \chi^{(3)}$
(from perturbation theory)

$|s|^2$ = power

$|a|^2$ = energy

$$\frac{da}{dt} = -i(\omega_0 - \alpha|a|^2)a - \frac{2}{\tau}a + \sqrt{\frac{2}{\tau}}s_{1+}$$

$$s_{1-} = -s_{1+} + \sqrt{\frac{2}{\tau}}a, \quad s_{2-} = \sqrt{\frac{2}{\tau}}a$$

gives cubic equation
for transmission
… bistable curve

TCMT + Perturbation Theory

SPM = small change in refractive index

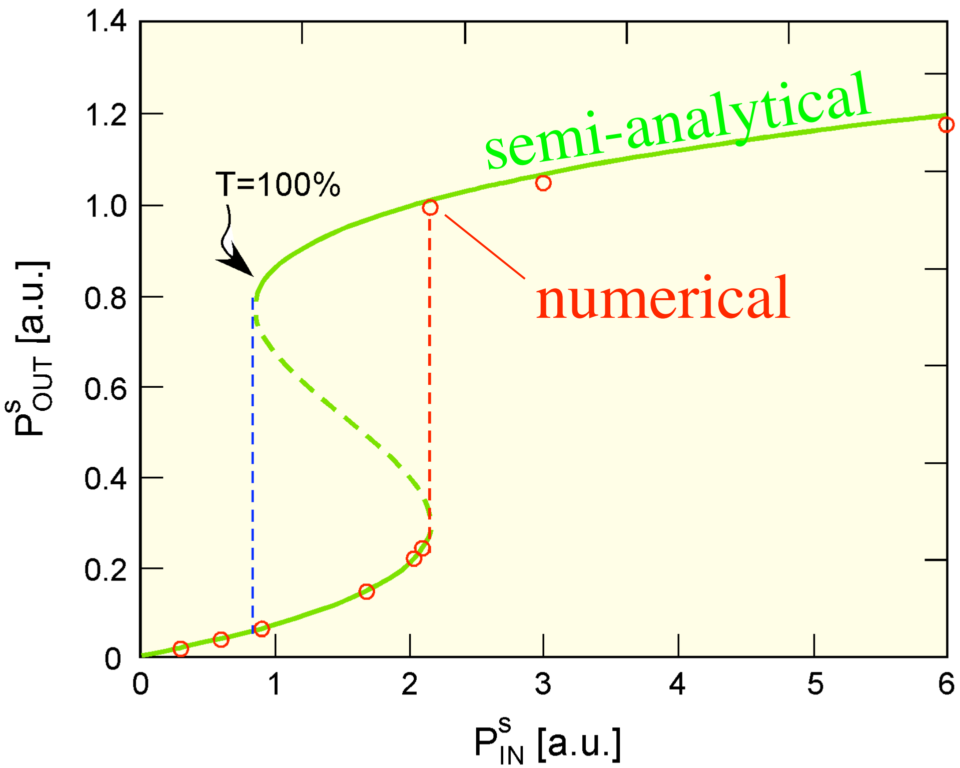
… evaluate $\Delta\omega$ by 1st-order perturbation theory

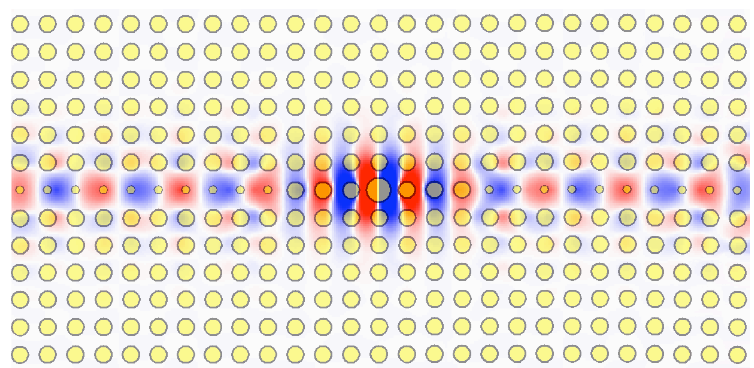
$$\alpha_{ii} = \frac{1}{8} \frac{\int d^3\mathbf{x}\ \varepsilon\chi^{(3)} \left|\mathbf{E}_i \cdot \mathbf{E}_i\right|^2 + \left|\mathbf{E}_i \cdot \mathbf{E}_i^*\right|^2}{\left[\int d^3\mathbf{x}\ \varepsilon \left|\mathbf{E}_i\right|^2\right]^2}$$

$\Rightarrow$ all relevant parameters (ω, τ or Q, α) can be computed from the resonant mode of the linear system

Accuracy of Coupled-Mode Theory

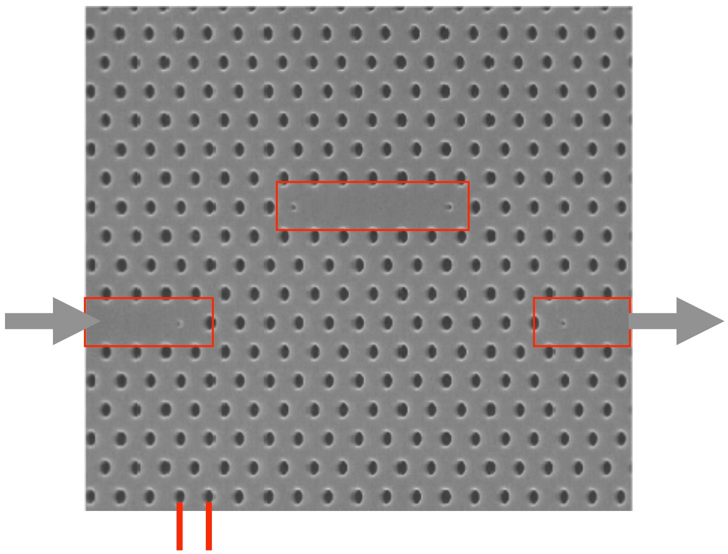
[Soljacic *et al*., *PRE Rapid*. *Comm*. **66**, 055601 (2002).]





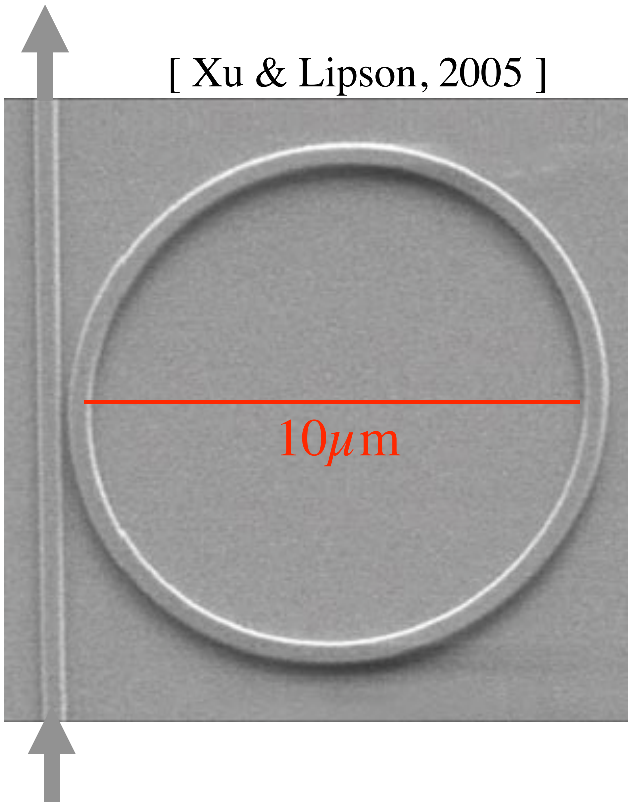
Optical Bistability in Practice

[Notomi *et al*. (2005).]



Q ~ 30,000
V ~ 10 optimum
Power threshold ~ 40 μW

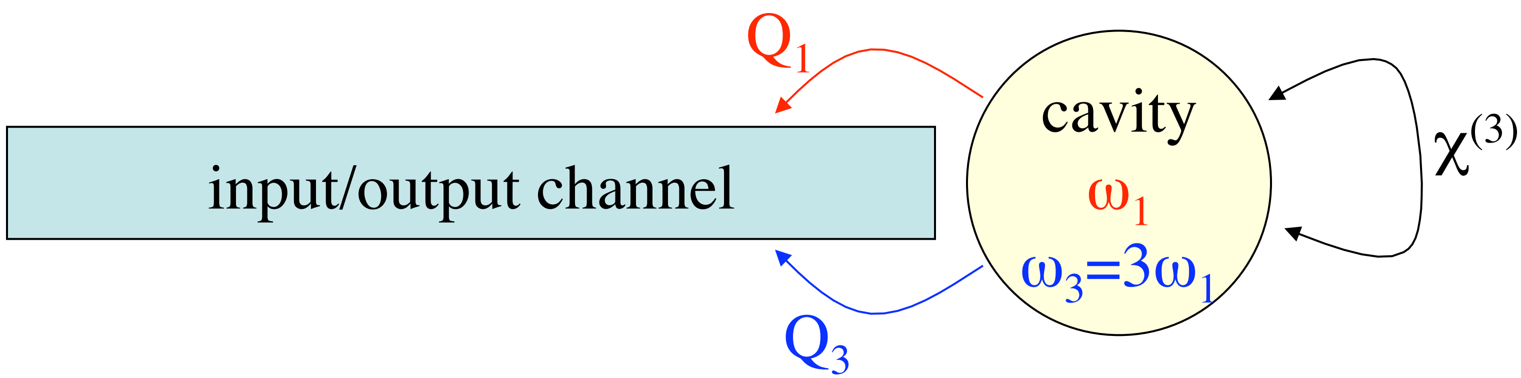
[Xu & Lipson, 2005]

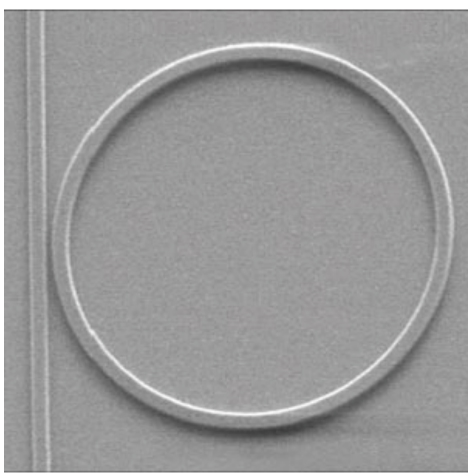


Q ~ 10,000
V ~ 300 optimum
Power threshold ~ 10 mW

THG in Doubly-Resonant Cavities

[publications from our group: H. Hashemi (2008) & A. Rodriguez (2007)]





e.g. ring resonator
with proper geometry

Not easy to make at micro-scale

— must precisely tune ω_3 / ω_1

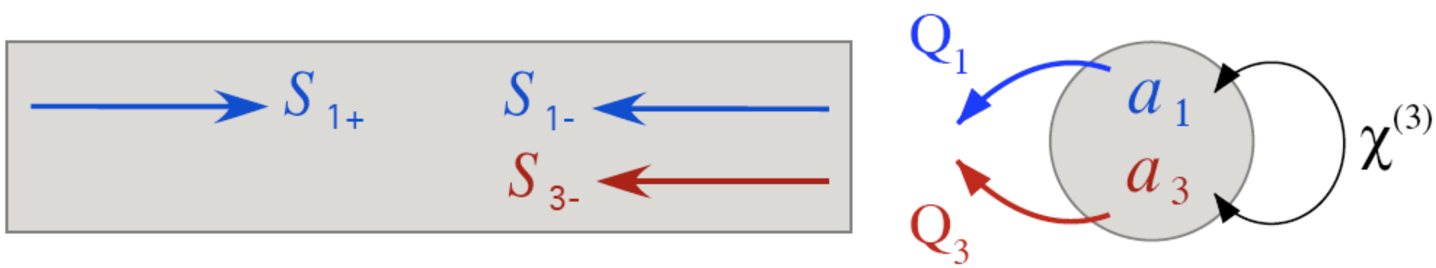
— materials must be ok at ω_1 and $3\omega_1$

But … what if we could do it?

… what are the consequences?

Coupled-mode Theory for THG

third harmonic generation



SPM XPM down-conversion

$$\frac{da_1}{dt} = \left(i\omega_1\left(1-\alpha_{11}|a_1|^2-\alpha_{13}|a_3|^2\right)-\frac{1}{\tau_1}\right)a_1 - i\omega_1\beta_1(a_1^*)^2a_3+\sqrt{\frac{2}{\tau_{s,1}}}s_+$$

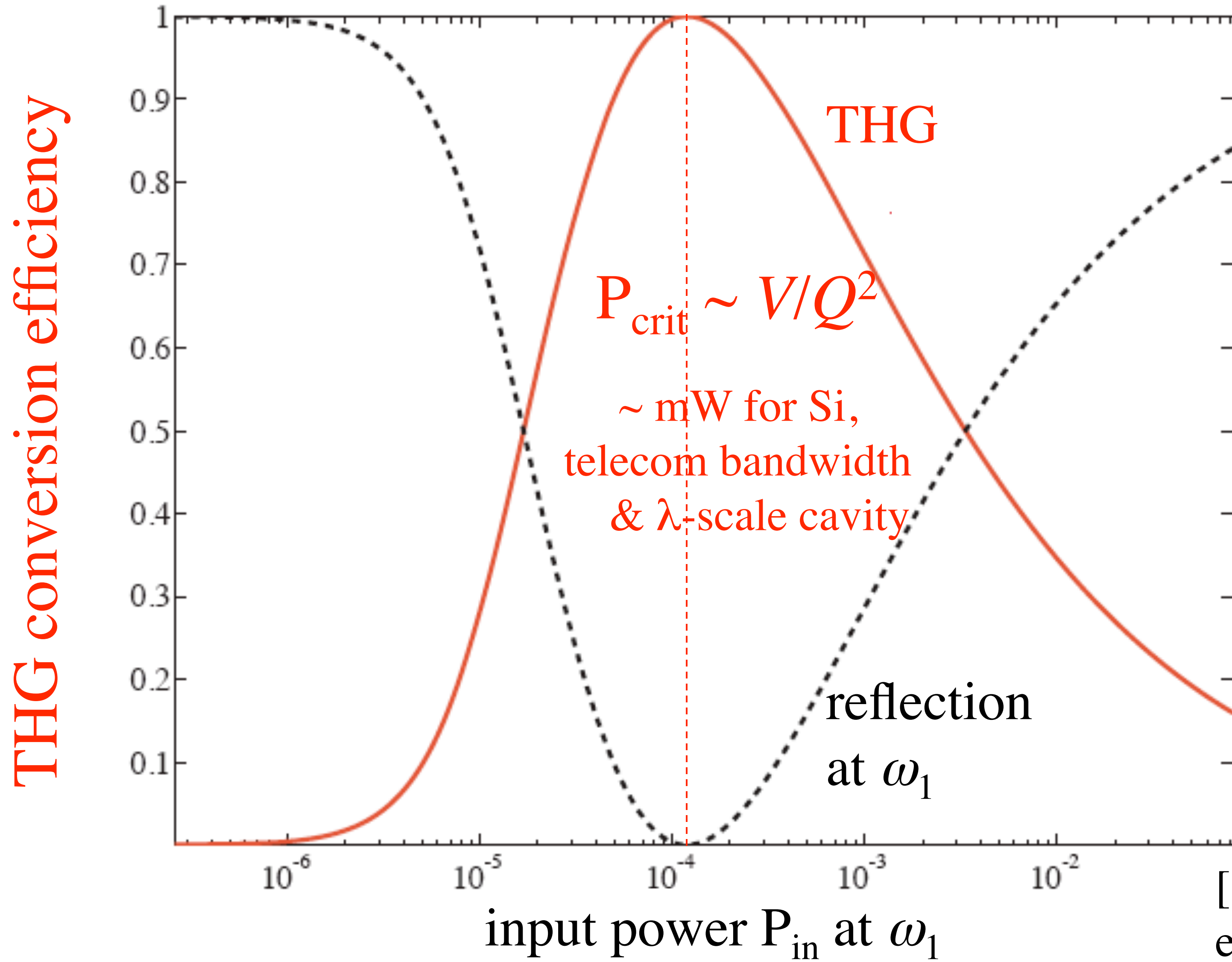
$$\frac{da_3}{dt} = \left(i\omega_3\left(1-\alpha_{33}|a_3|^2-\alpha_{31}|a_1|^2\right)-\frac{1}{\tau_3}\right)a_3 - i\omega_3\beta_3a_1^3+\sqrt{\frac{2}{\tau_{s,3}}}s_+$$

SPM XPM THG

[Rodriguez et al. (2007)]

α=0: Critical Power for Efficient THG

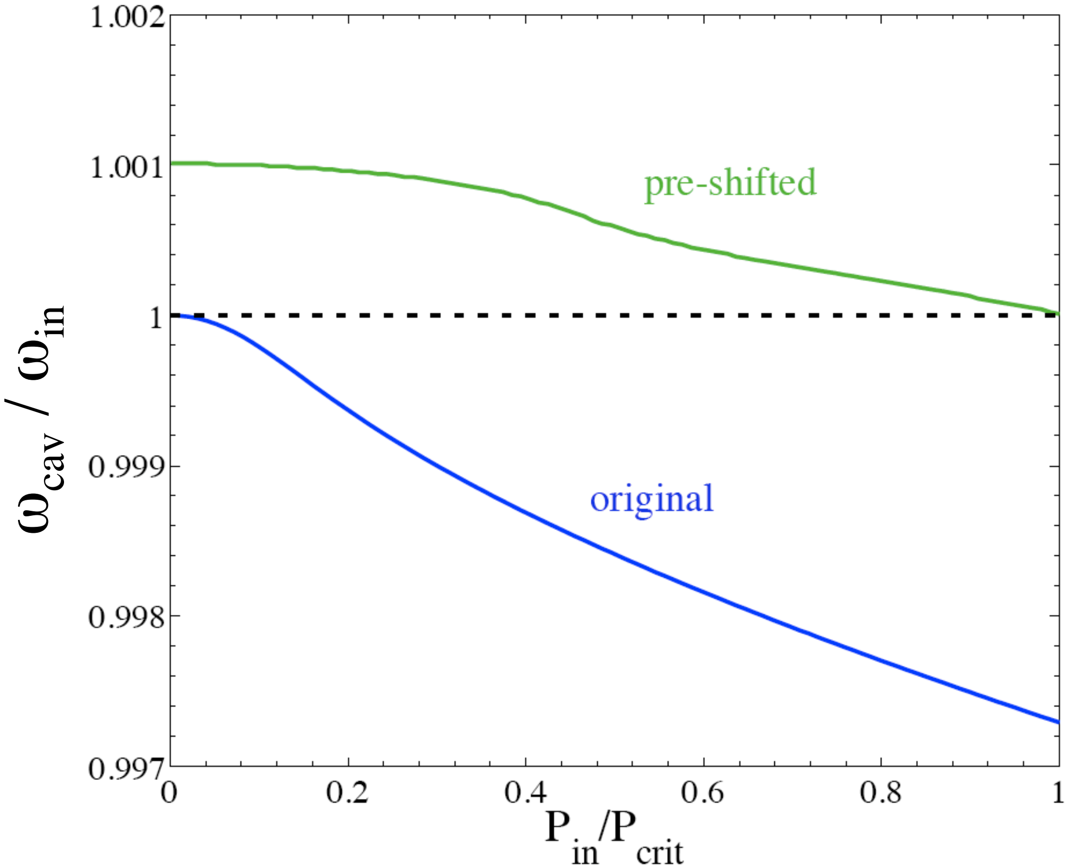
third-harmonic generation in doubly-resonant $\chi^{(3)}$ (Kerr) cavity



[Rodriguez et al. (2007)]

Detuning for Kerr THG

[Hashemi et al (2008)]



because of SPM/XPM, the input power changes resonant w …

compensate by pre-shifting resonance so that at $P_{in} = P_{crit}$ we have $\omega_3 = 3\ \omega_1$

Stability and Dynamics?

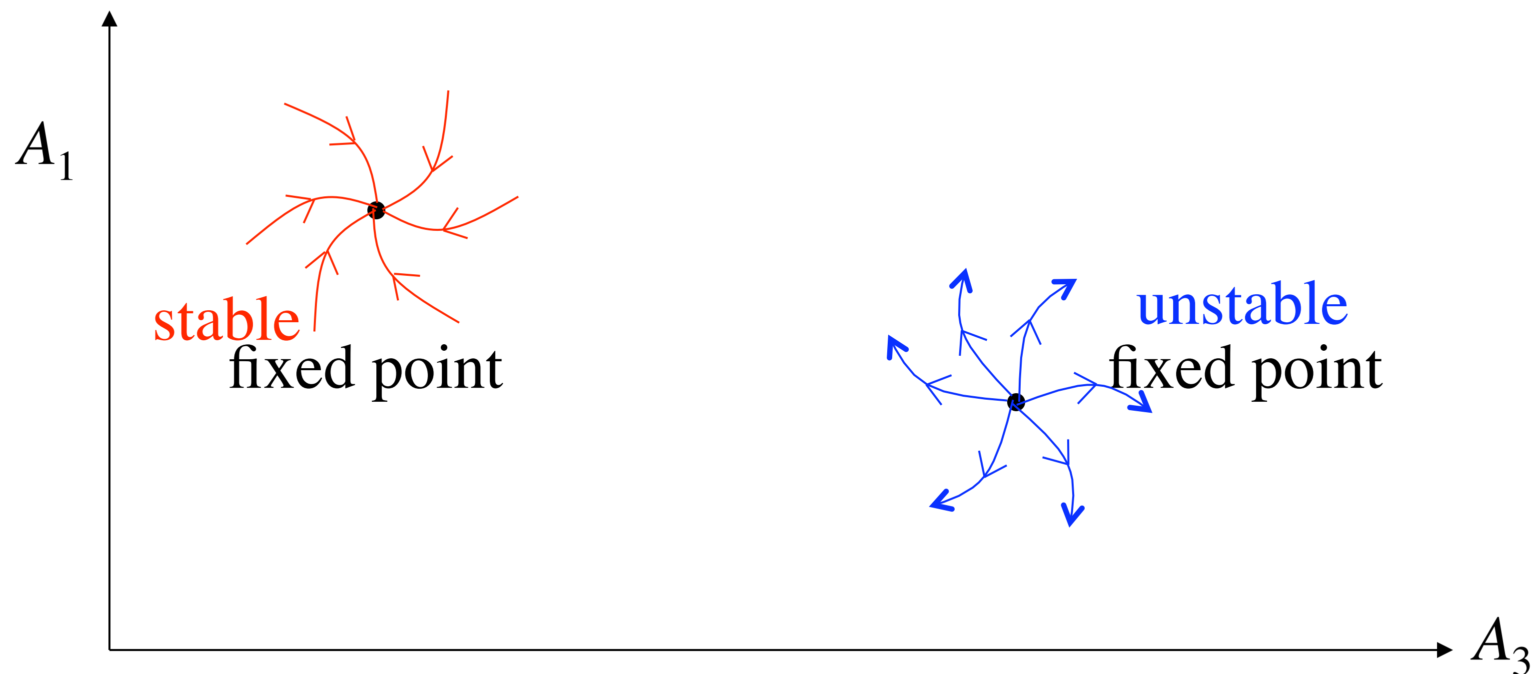
brief review

Steady state-solution: a_1 oscillating at ω_1, a_3 at ω_3

— rewrite equations in terms of $A_1 = a_1\, e^{i\omega_1 t}$

$A_3 = a_3\, e^{i\omega_3 t}$

then steady state = A_1, A_3 *constant* = fixed-point

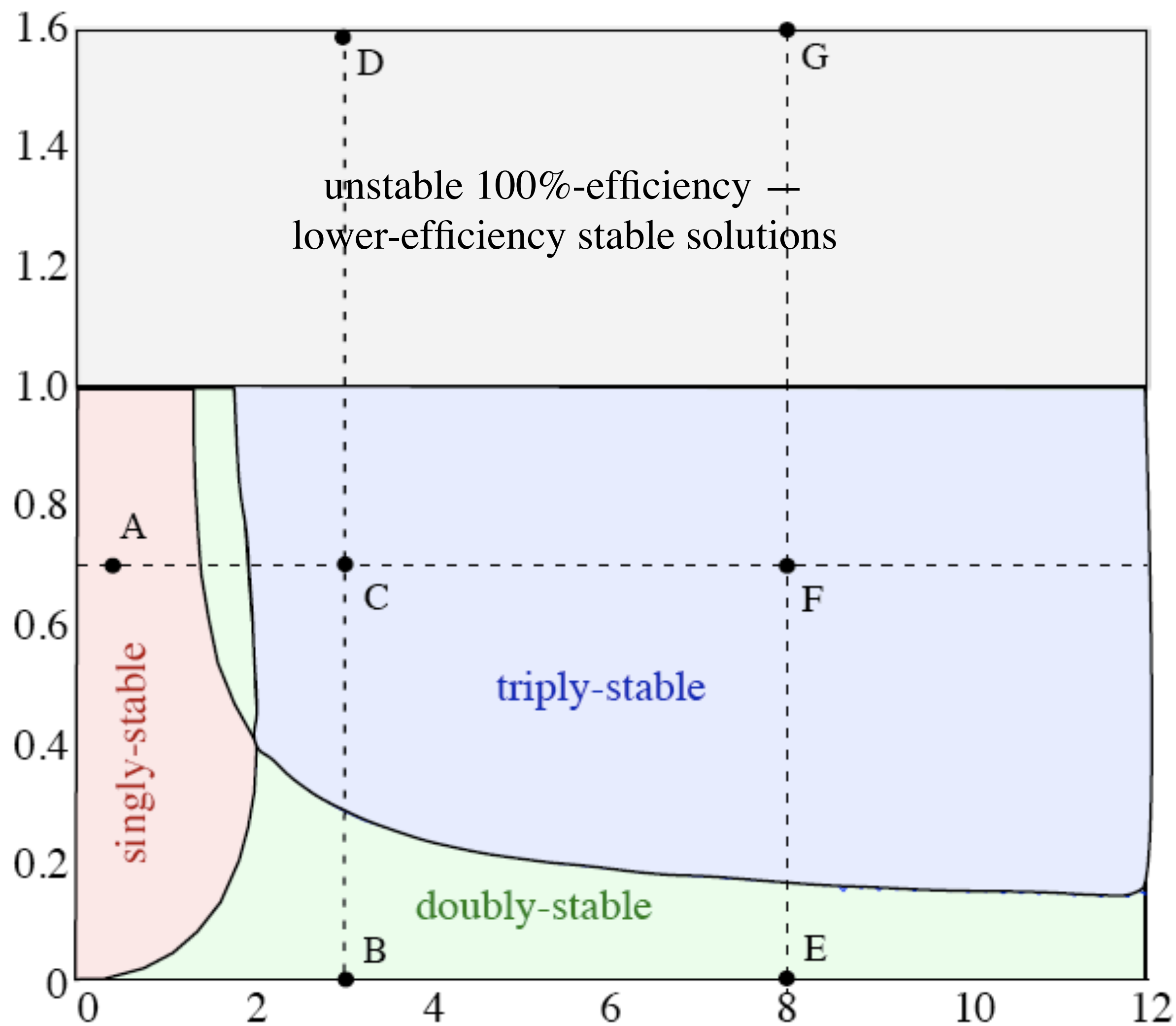


cartoon phase space (A_1, A_3 are actually complex) *for simplicity*, assume SPM = XPM coefficients:

$$\alpha_{11} = \alpha_{33} = \alpha_{13} = \alpha_{31} = \alpha$$

THG Stability Phase Diagram

[Hashemi et al (2008)]



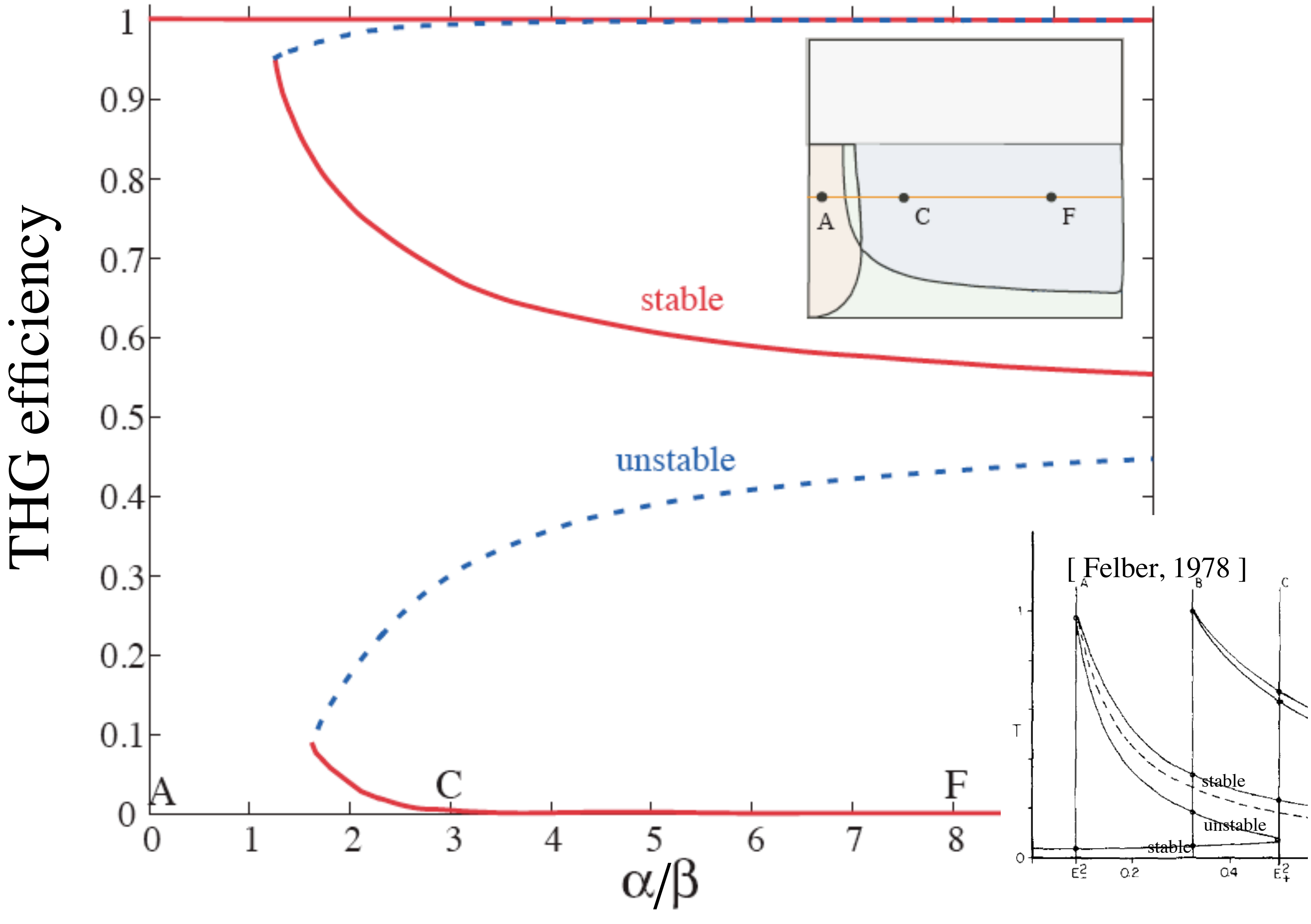
$$\frac{Q_3}{3Q_1} = \frac{\tau_3}{\tau_1}$$

α/β_1

SPM+XPM / THG

Bifurcation vs. SPM/XPM

[Hashemi et al (2008)]



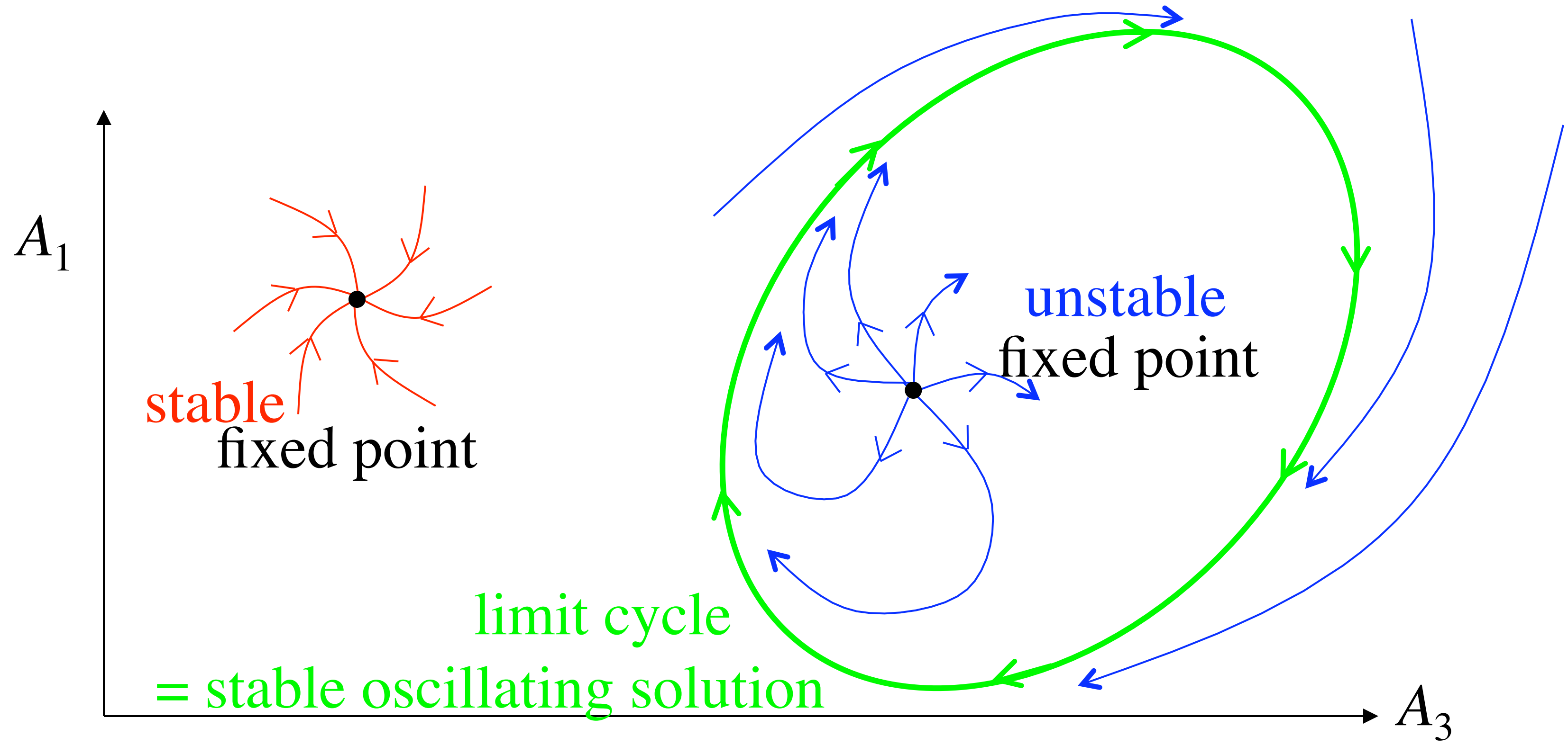
Limit Cycles

Steady state-solution: a_1 oscillating at ω_1, a_3 at ω_3

— rewrite equations in terms of $A_1 = a_1\, e^{i\omega_1 t}$

$A_3 = a_3\, e^{i\omega_3 t}$

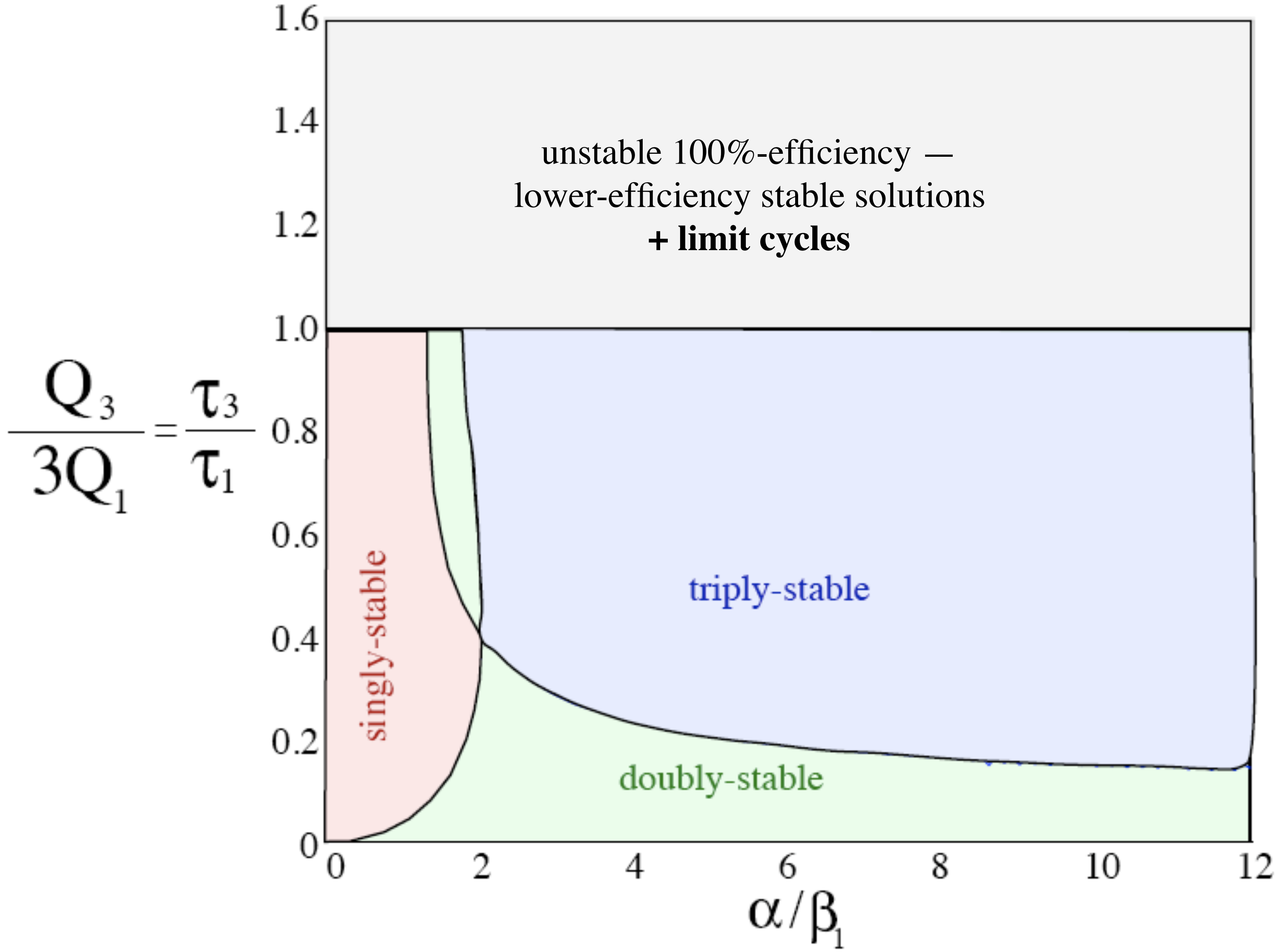
then steady state = A_1, A_3 *constant* = fixed-point



cartoon phase space (A_1, A_3 are actually complex)

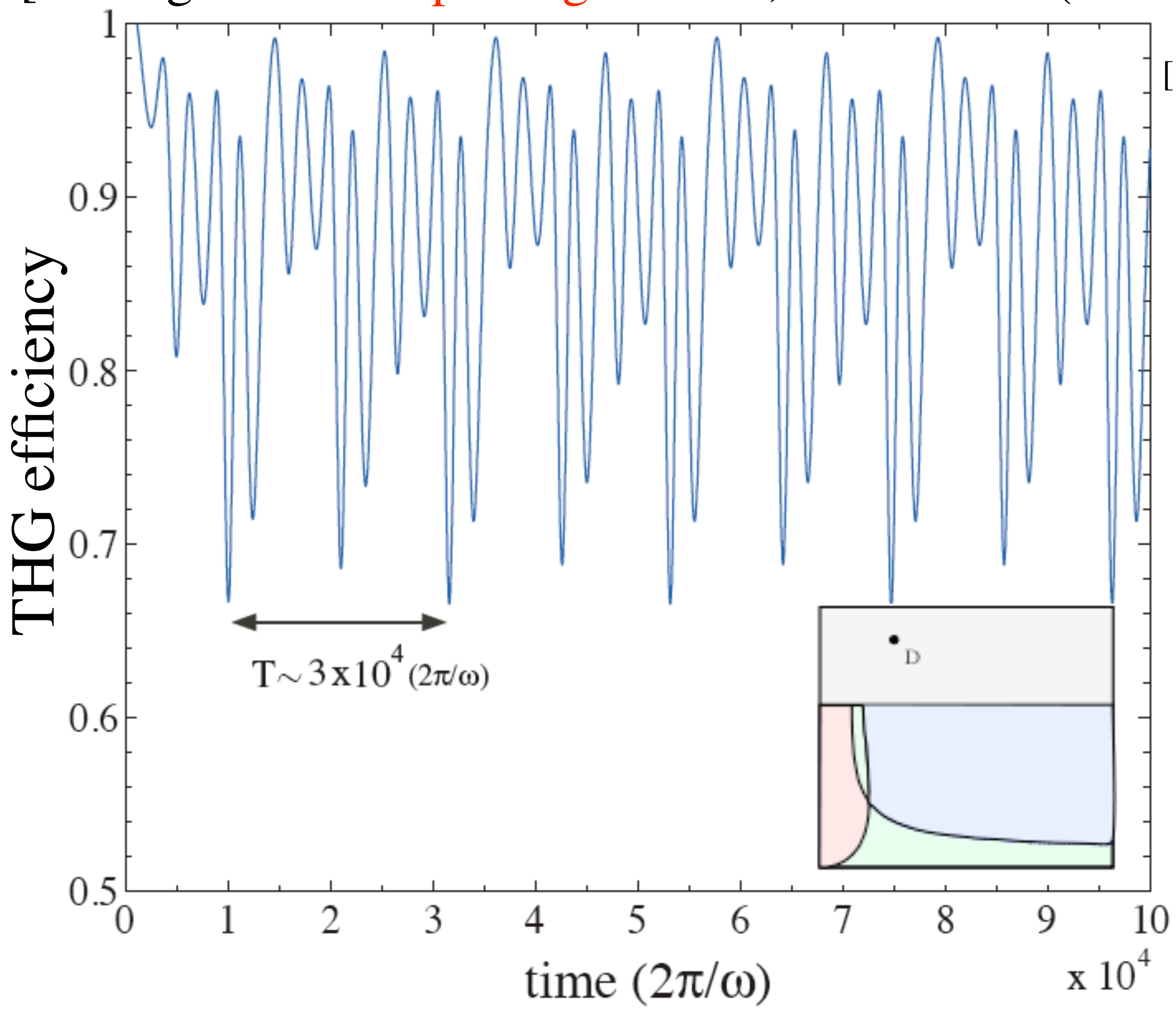
Stability Phase Diagram

[Hashemi et al (2008)]



An Optical Kerr-THG Oscillator

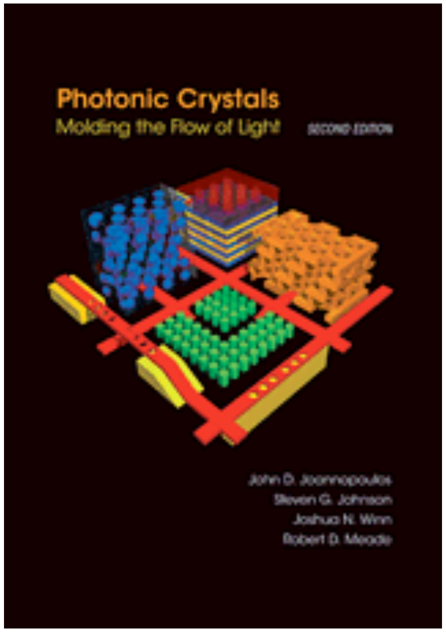
[analogous to self-pulsing in SHG; Drummond (1980)]



[Hashemi et al (2008)]

Summary: a rich set of behaviors is possible by coupling resonances, with powerful numerical & analytical tools…

to be continued…



Further reading:

Photonic Crystals book: http://jdj.mit.edu/book
(covers coupled-mode theory etc.)

Free FDTD software: http://jdj.mit.edu/meep
& tutorials

PML notes:
http://math.mit.edu/~stevenj/18.369/pml.pdf