



**The Abdus Salam
International Centre for Theoretical Physics**



2145-22

Spring College on Computational Nanoscience

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Computational Photonics: Cavities and Resonant Devices

S. JOHNSON

*MIT, Applied Mathematics
Cambridge, MA
USA*

Computational Nanophotonics: Cavities and Resonant Devices

Steven G. Johnson

MIT Applied Mathematics

Resonance

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

frequency ω_0

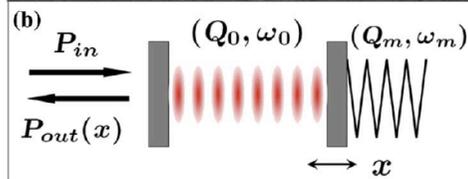
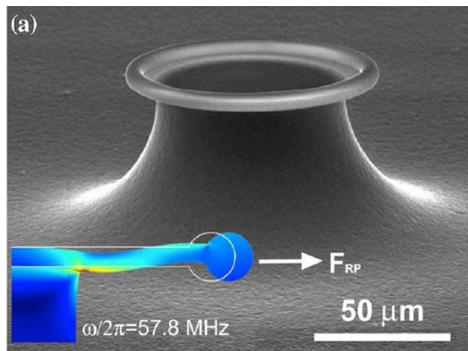
lifetime $\tau \gg 2\pi/\omega_0$

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

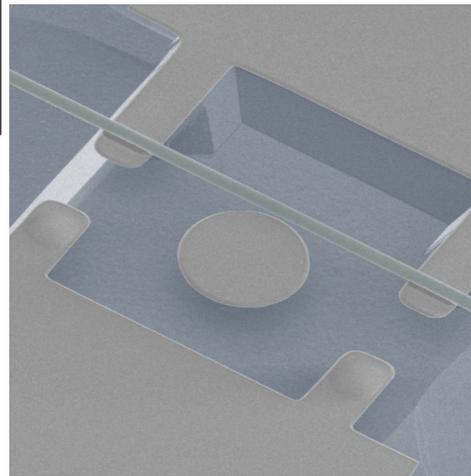
modal
volume V

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

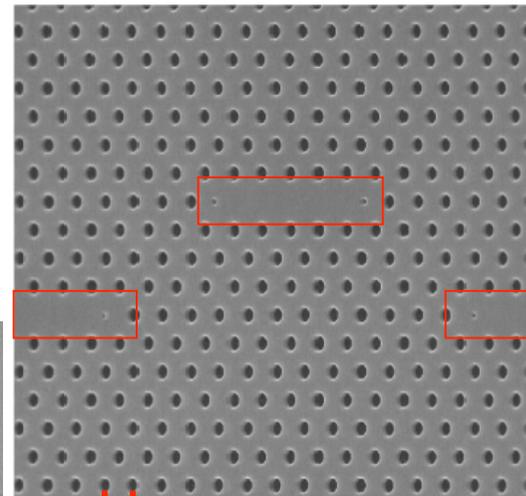
[Notomi *et al.* (2005).]



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

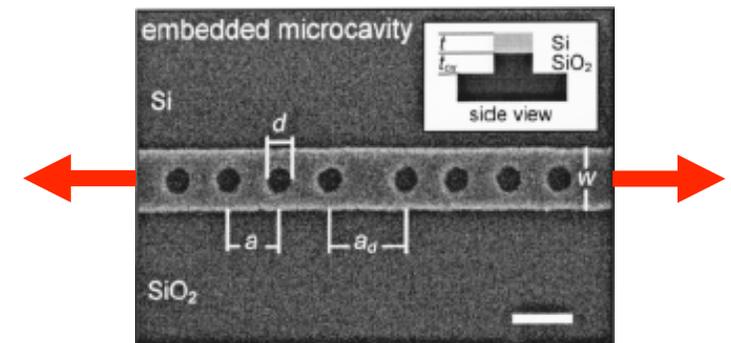


[Eichenfield *et al.* *Nature Photonics* **1**, 416 (2007)]



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, ...

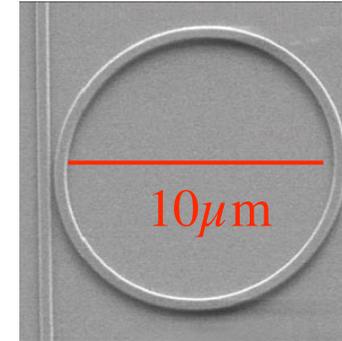
How Resonance?

need **mechanism** to trap light for long time



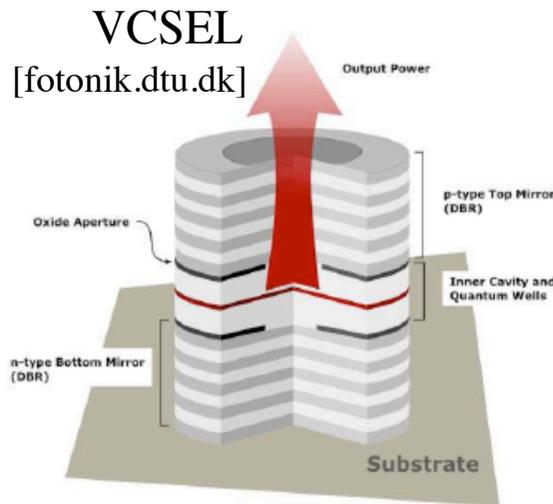
[llnl.gov]

metallic cavities:
good for microwave,
dissipative for infrared



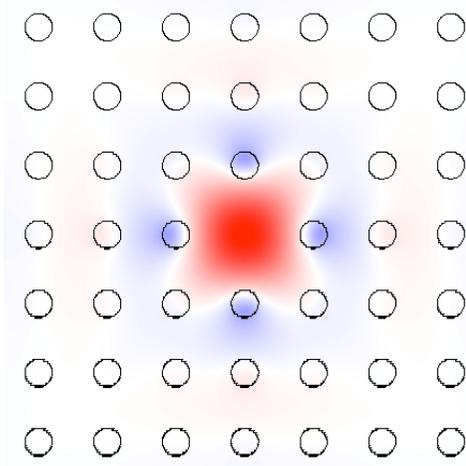
[Xu & Lipson (2005)]

ring/disc/sphere resonators:
a waveguide bent in circle,
bending loss $\sim \exp(-\text{radius})$



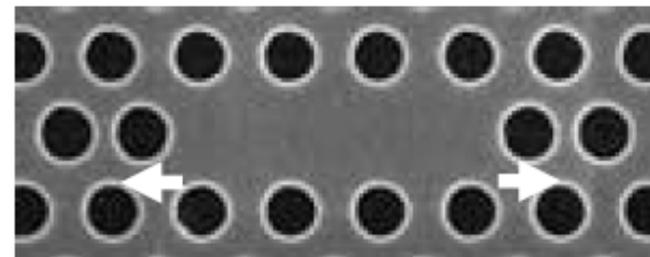
VCSEL

[fotonik.dtu.dk]



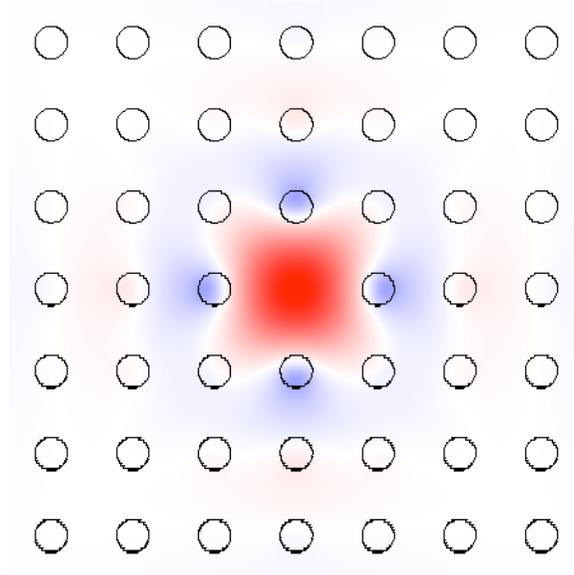
photonic bandgaps
(complete or partial
+ index-guiding)

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



(planar Si slab)

Microcavity Blues

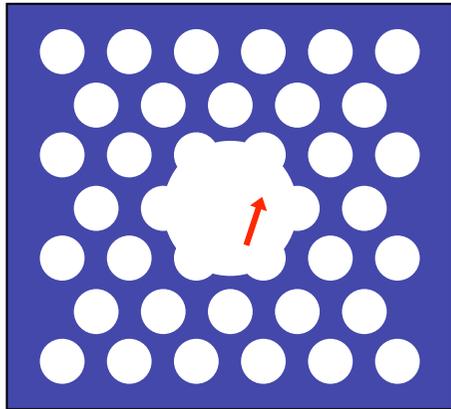


For cavities (*point defects*)
frequency-domain has its drawbacks:

- 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*

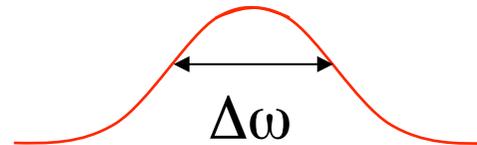
Time-Domain Eigensolvers

(finite-difference time-domain = FDTD)



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

- Excite with broad-spectrum **dipole** (\uparrow) source



tricky

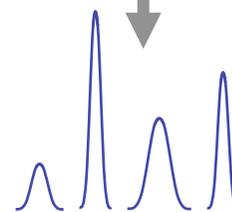
signal processing

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

complex ω_n



decay rate in time gives **loss**



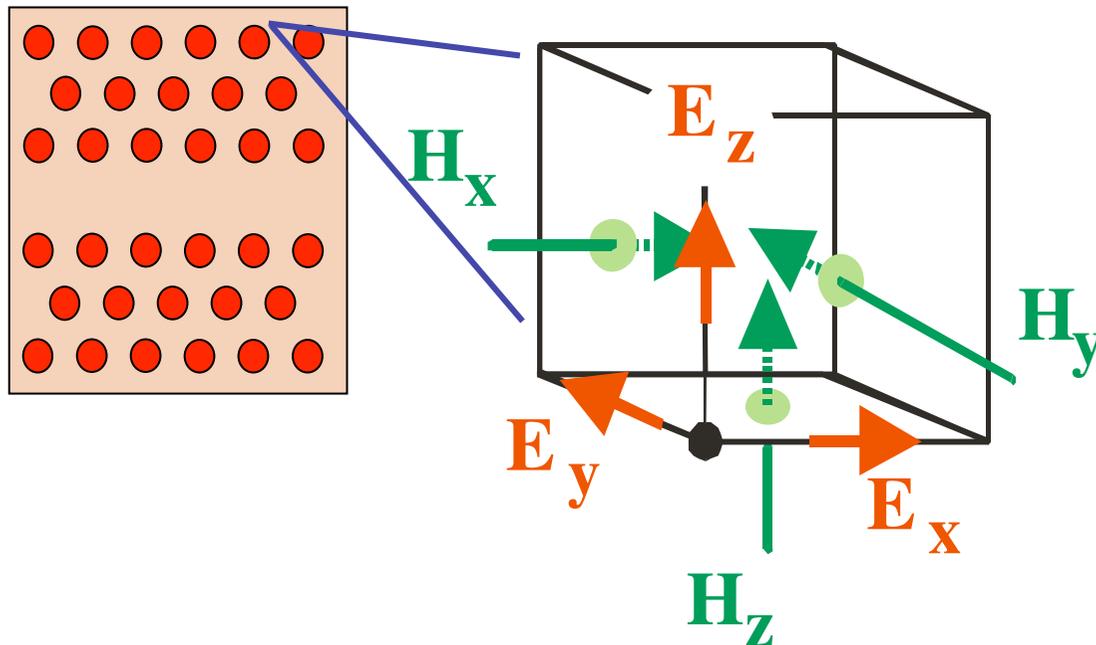
Response is many
sharp peaks,
one peak per mode

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

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

$$\mathbf{D} = \epsilon \mathbf{E} \quad \mathbf{B} = \mu \mathbf{H}$$



K.S. Yee 1966

A. Taflove & S.C. Hagness 2005

FDTD: Yee leapfrog algorithm

2d example:

1) at time t : Update \mathbf{D} fields everywhere

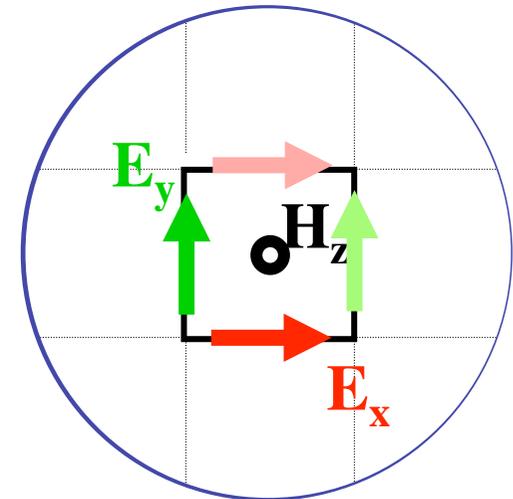
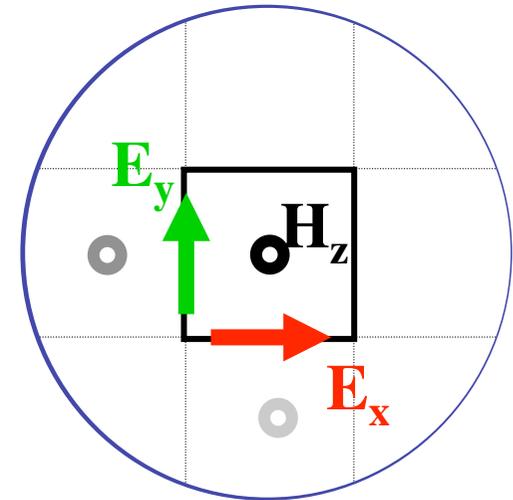
using spatial derivatives of \mathbf{H} , then find $\mathbf{E} = \epsilon^{-1} \mathbf{D}$ (ϵ constant)

$$\mathbf{E}_x += \frac{\Delta t}{\epsilon \Delta y} \left(\mathbf{H}_z^{j+0.5} - \mathbf{H}_z^{j-0.5} \right)$$

$$\mathbf{E}_y -= \frac{\Delta t}{\epsilon \Delta x} \left(\mathbf{H}_z^{i+0.5} - \mathbf{H}_z^{i-0.5} \right)$$

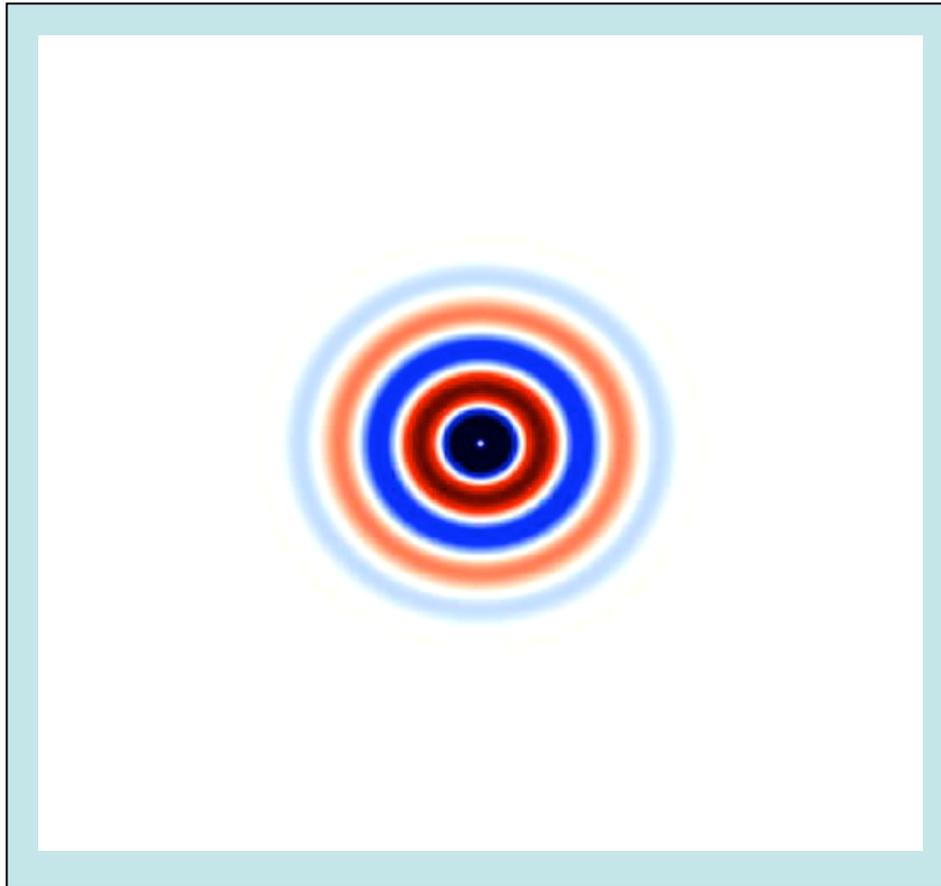
2) at time $t+0.5$: Update \mathbf{H} fields everywhere using spatial derivatives of \mathbf{E} (μ constant)

$$\mathbf{H}_z += \frac{\Delta t}{\mu} \left(\frac{\mathbf{E}_x^{j+1} - \mathbf{E}_x^j}{\Delta y} + \frac{\mathbf{E}_y^i - \mathbf{E}_y^{i+1}}{\Delta x} \right)$$



Why Absorbers?

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



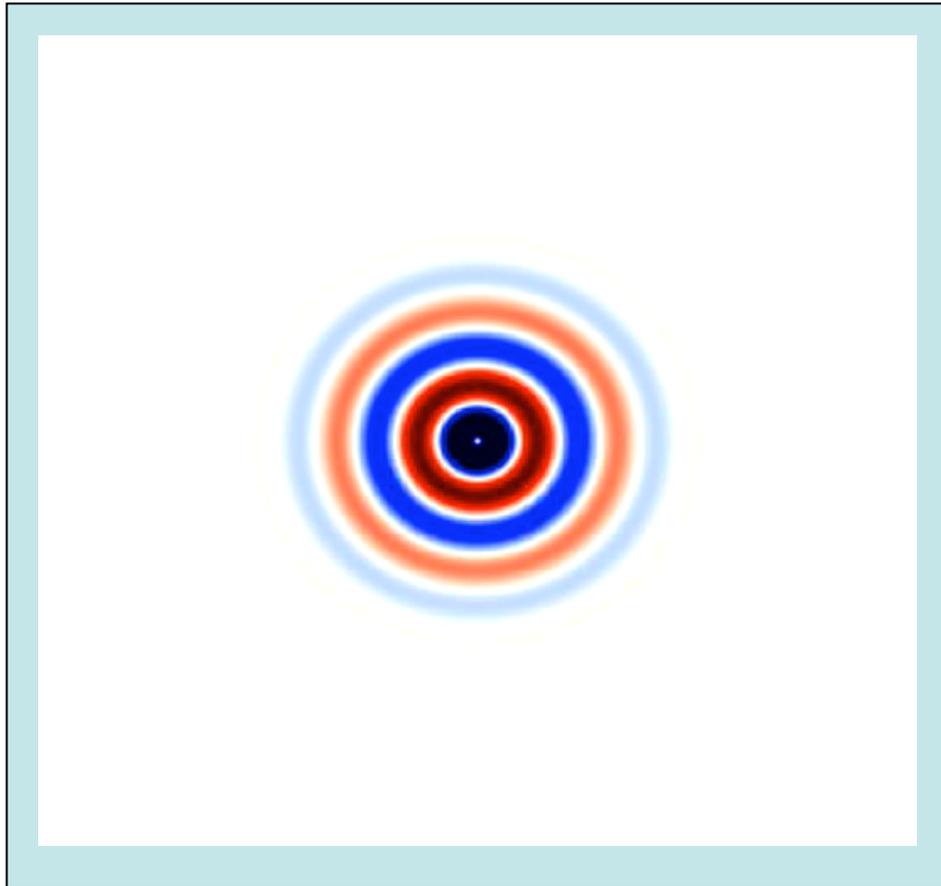
In a wave equation, a hard-wall **truncation** gives **reflection artifacts**.

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.

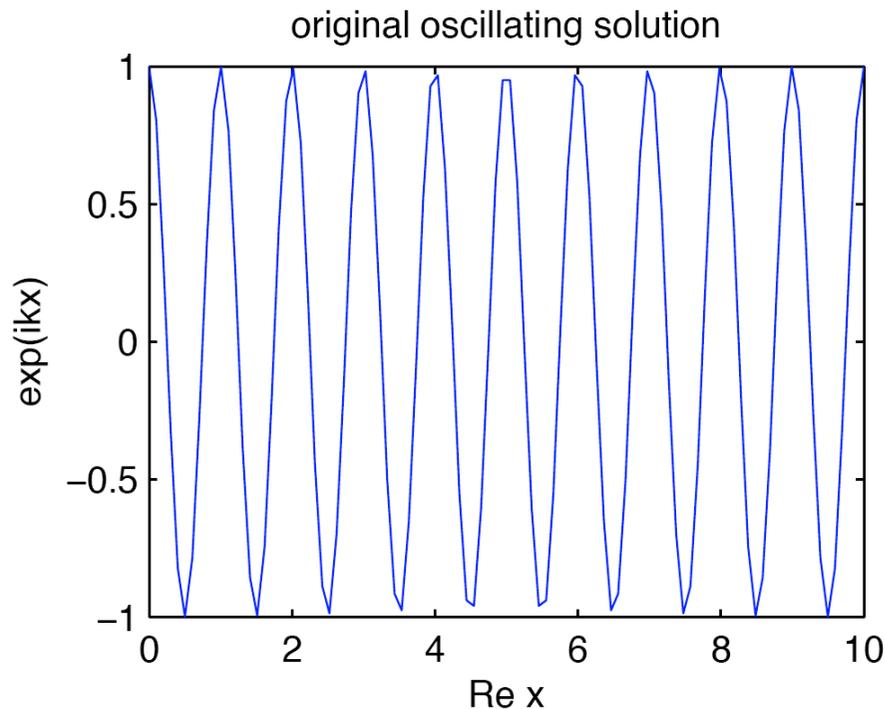
Several derivations, cleanest
& most general via “**complex
coordinate stretching**”

[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 $\omega > 0$.

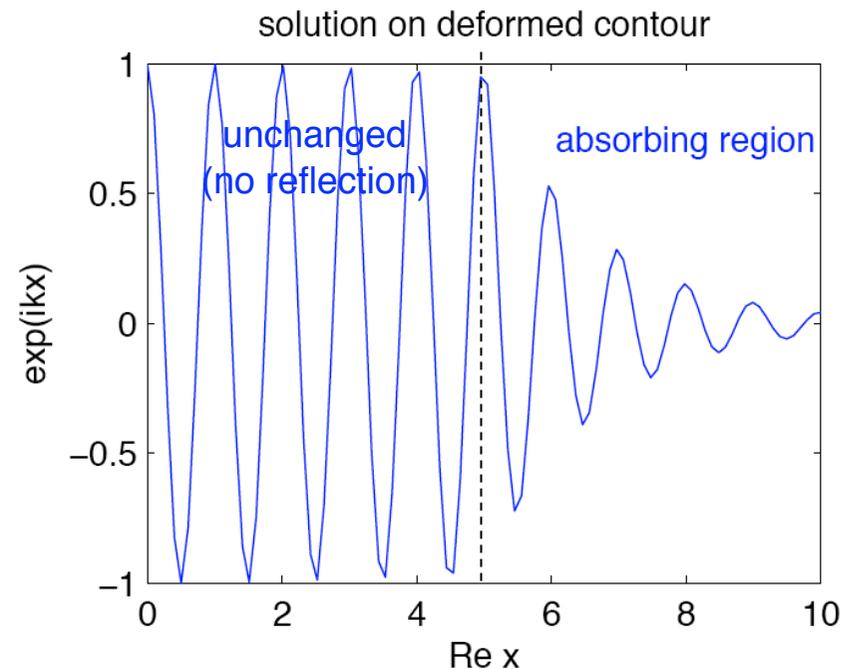
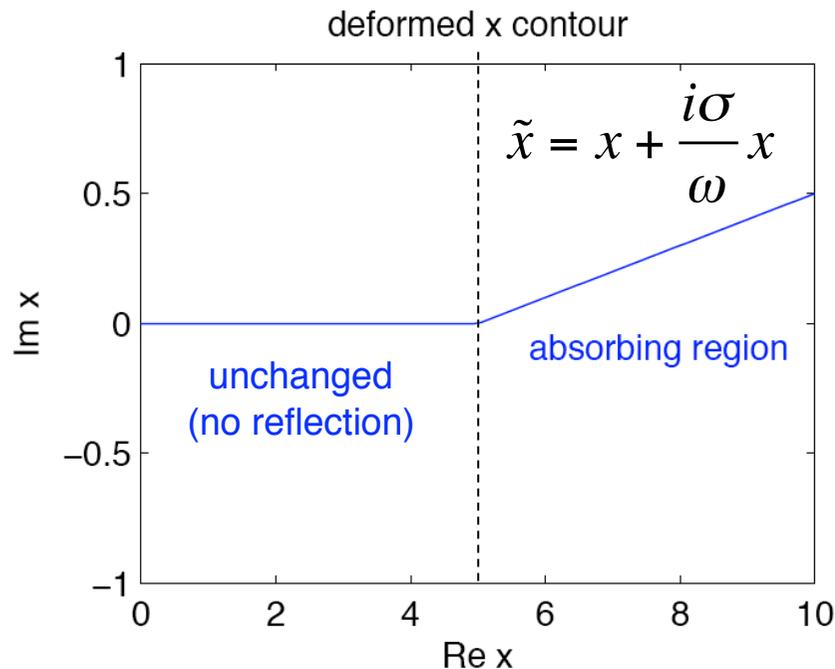
$$\text{fields} \sim f(y, z) e^{i(kx - \omega t)} \quad (\text{usually, } k > 0)$$



(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



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

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)

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

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

nondispersive materials: $k/\omega \sim \text{constant}$
 \Rightarrow decay rate independent of ω

PML Step 3: Effective materials

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

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

x PML Jacobian

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

$$\begin{pmatrix} \partial x \\ \partial \tilde{x} \end{pmatrix}$$

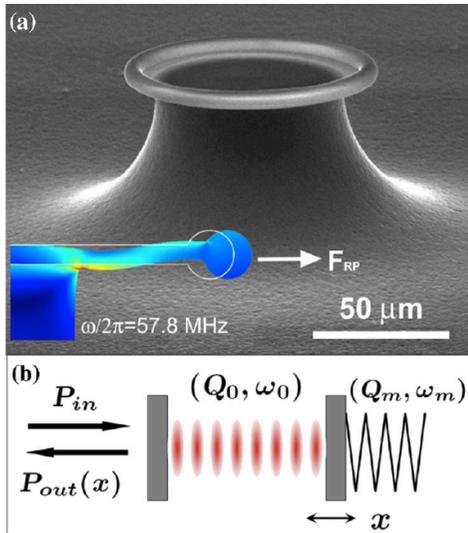
for isotropic starting materials:

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

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**

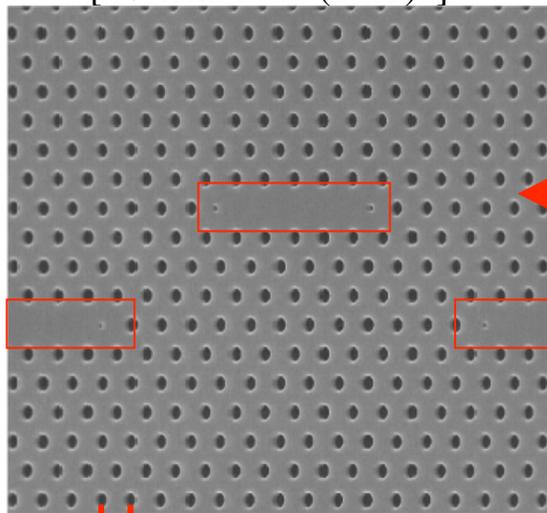
“Temporal coupled-mode theory”

- 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 \Rightarrow 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)

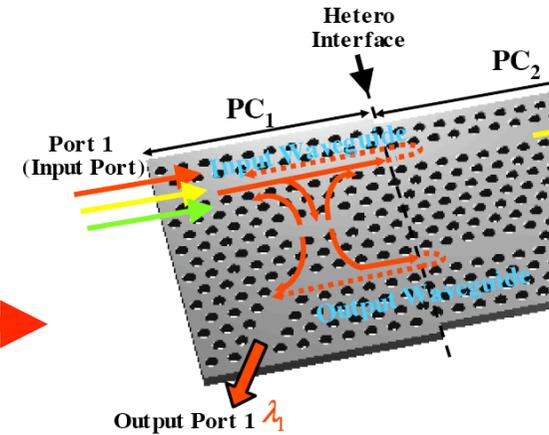
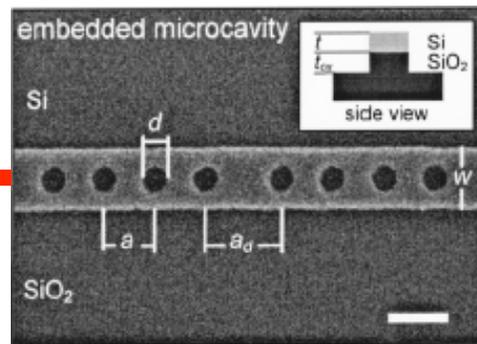
TCMT example: a linear filter

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

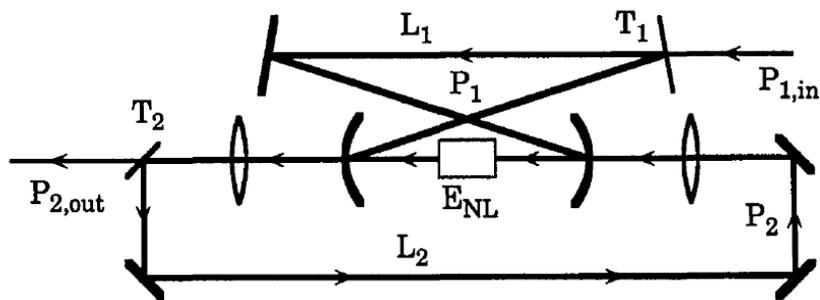


420 nm

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



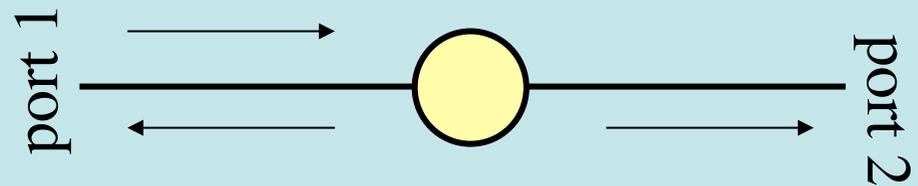
[Takano *et al.* (2006)]



[Ou & Kimble (1993)]

= abstractly:

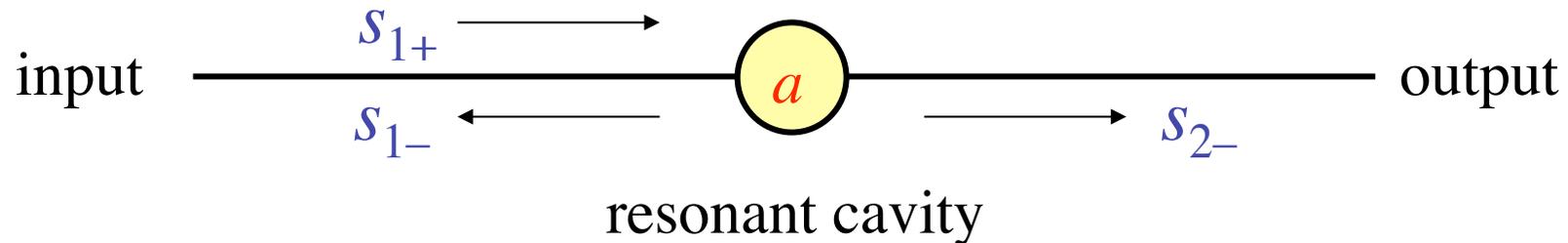
two single-mode i/o ports
+ one resonance



resonant cavity
frequency ω_0 , lifetime τ

Temporal Coupled-Mode Theory

for a linear filter



resonant cavity
frequency ω_0 , lifetime τ

$|s|^2 = \text{power}$

$|a|^2 = \text{energy}$

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

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

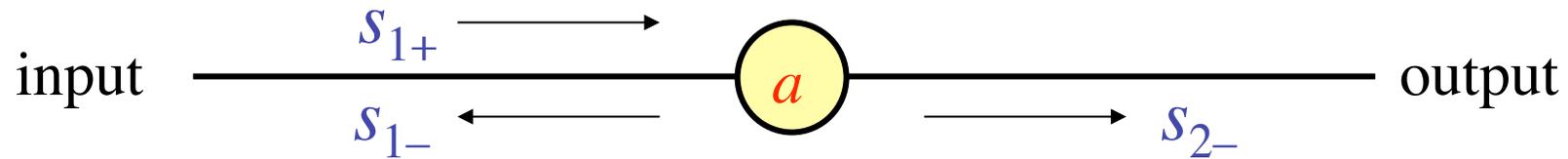
can be relaxed

assumes only:

- exponential decay
(**strong confinement**)
- linearity
- conservation of energy
- time-reversal symmetry

Temporal Coupled-Mode Theory

for a linear filter

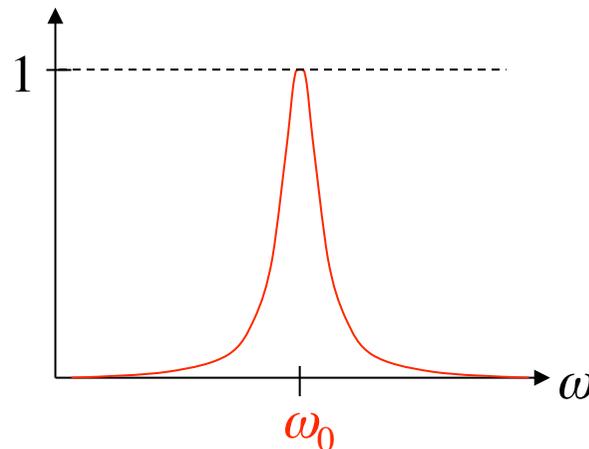


resonant cavity
frequency ω_0 , lifetime τ

$|s|^2 = \text{flux}$

$|a|^2 = \text{energy}$

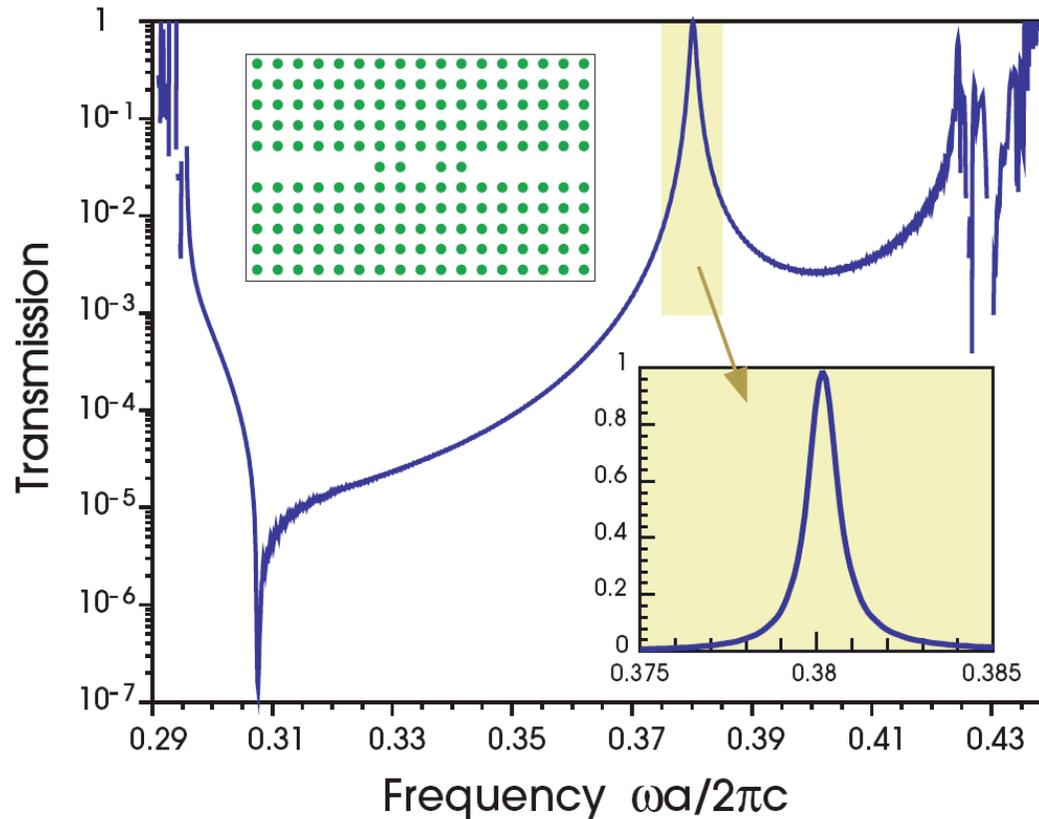
transmission T
 $= |s_{2-}|^2 / |s_{1+}|^2$



$T = \text{Lorentzian filter}$

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

Resonant Filter Example



Lorentzian peak, as predicted.

An apparent *miracle*:

~ 100% transmission
at the resonant frequency

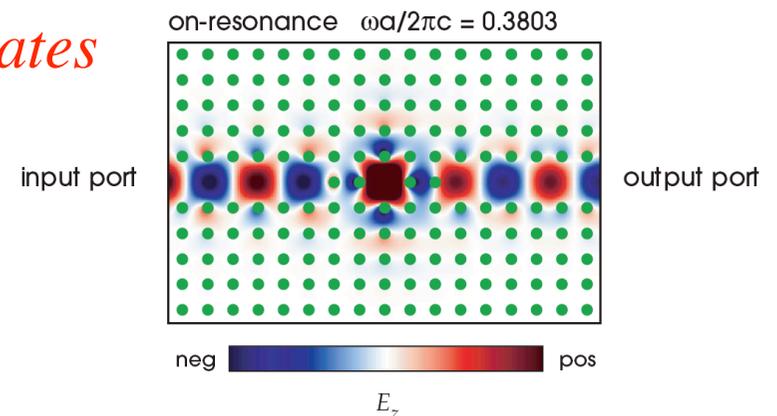
cavity decays to input/output with *equal rates*

⇒ At resonance, reflected wave

destructively interferes

with backwards-decay from cavity

& the two *exactly cancel*.



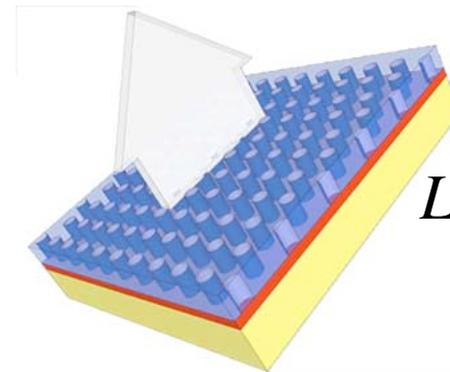
Some interesting resonant transmission processes



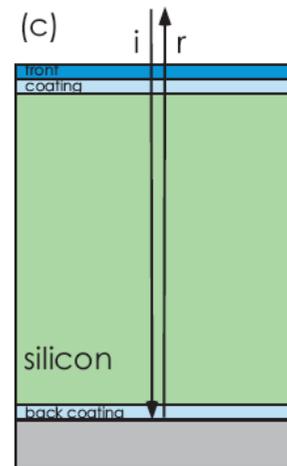
Wireless resonant power transfer

[M. Soljacic, MIT (2007)]

witricity.com



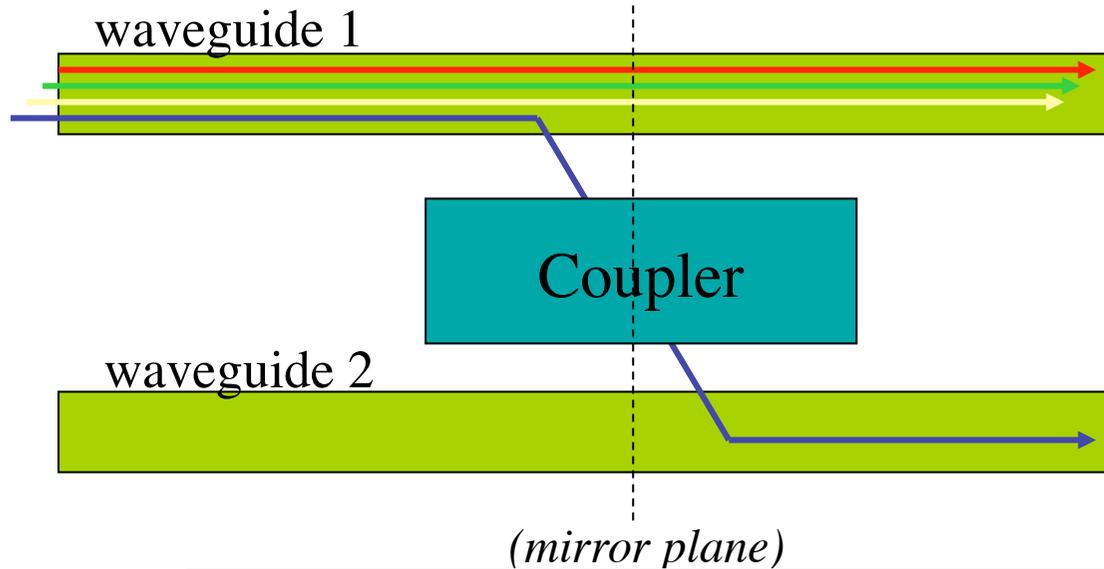
*Resonant
LED emission*
luminus.com



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

[e.g. Ghebrebrhan (2009)]

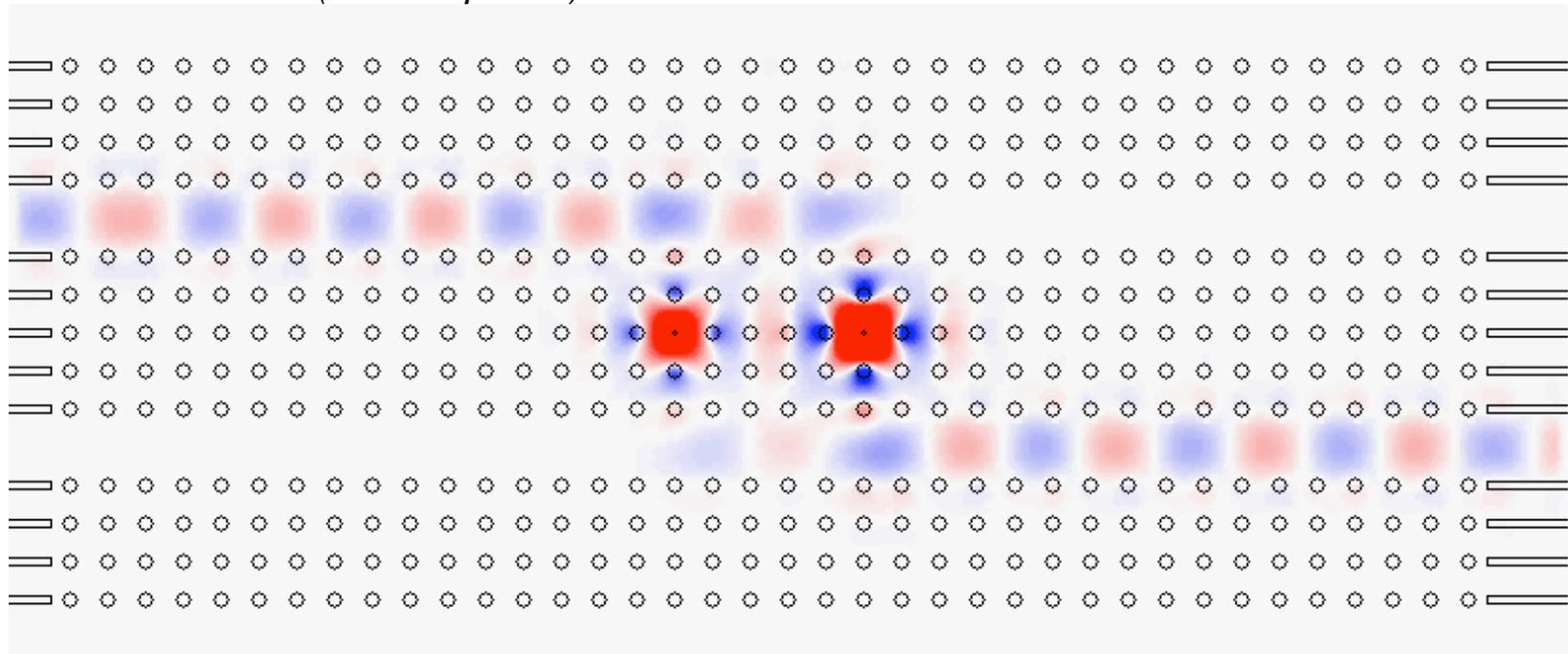
Another interesting example: Channel-Drop Filters



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

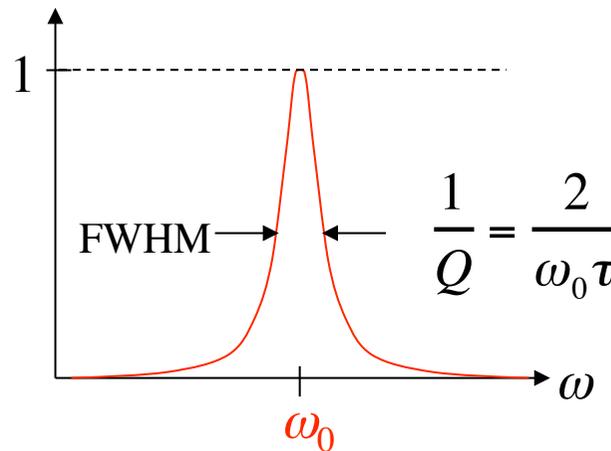
$$Q = \omega_0 \tau / 2$$

quality factor $Q = \#$ optical periods for energy to decay by $\exp(-2\pi)$

$$\text{energy} \sim \exp(-\omega_0 t / Q) = \exp(-2t / \tau)$$

in frequency domain: $1/Q = \text{bandwidth}$

*from temporal
coupled-mode theory:*



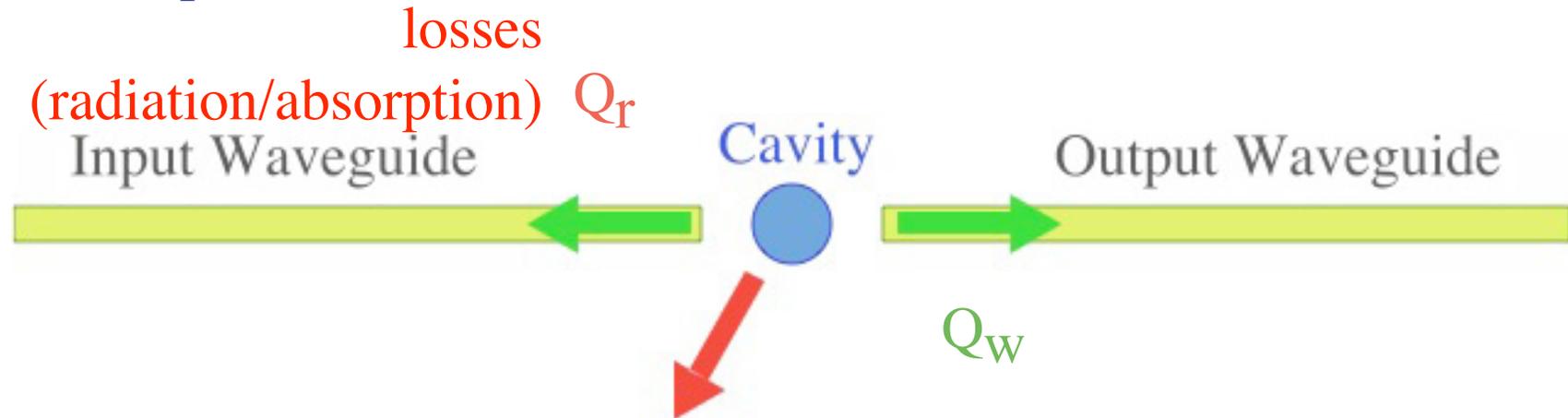
$T = \text{Lorentzian filter}$

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

...quality factor Q

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: $Q_r \gg Q_w$
TCMT \Rightarrow

$$1 - \text{transmission} \sim 2Q / Q_r$$

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

Nonlinearities + Microcavities?

weak effects

$$\Delta n < 1\%$$

very intense fields

& sensitive to small changes

A simple idea:

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

That's not all!

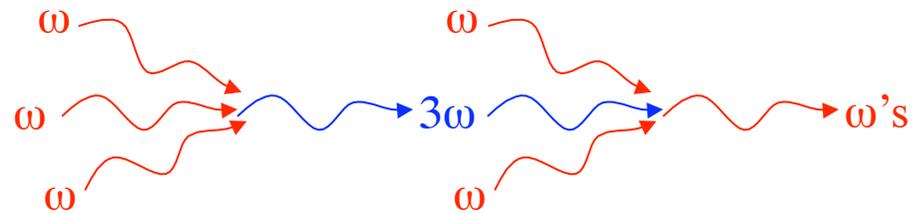
nonlinearities + microcavities

= *qualitatively* new phenomena

Nonlinear Optics

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

- Self-Phase Modulation (**SPM**)
= change in refractive index(ω) $\sim |\mathbf{E}(\omega)|^2$
- Cross-Phase Modulation (**XPM**)
= change in refractive index(ω) $\sim |\mathbf{E}(\omega_2)|^2$
- Third-Harmonic Generation (**THG**) & down-conversion (FWM)
= $\omega \rightarrow 3\omega$, and back
- etc...



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

- 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

$$\Delta n < 1\%$$

very intense fields

& sensitive to small changes

A simple idea:

for the same input power, nonlinear effects
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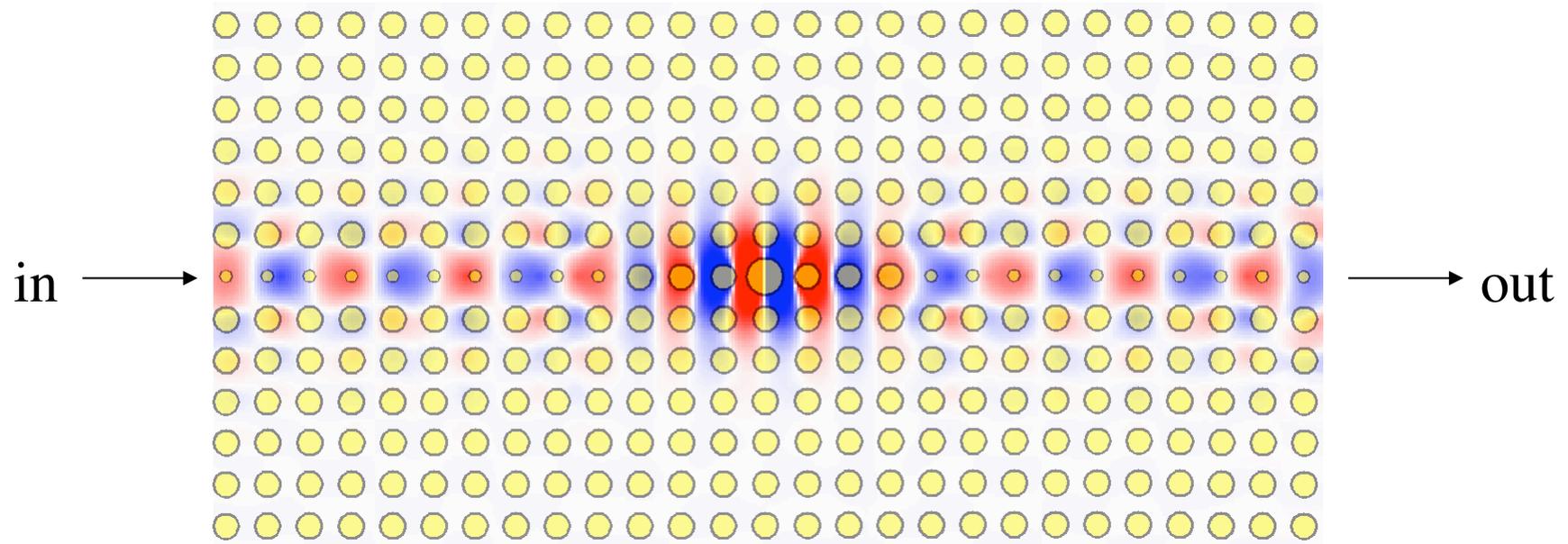
That's not all!

nonlinearities + microcavities

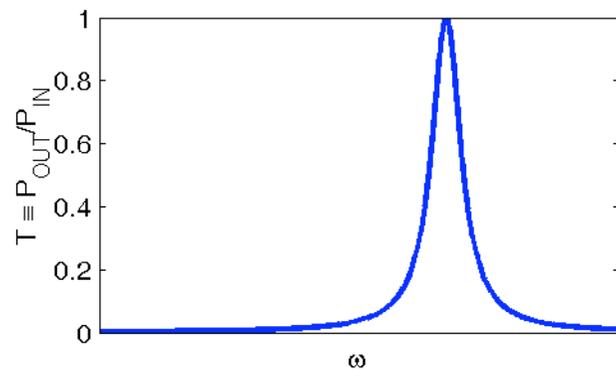
= *qualitatively* new phenomena

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

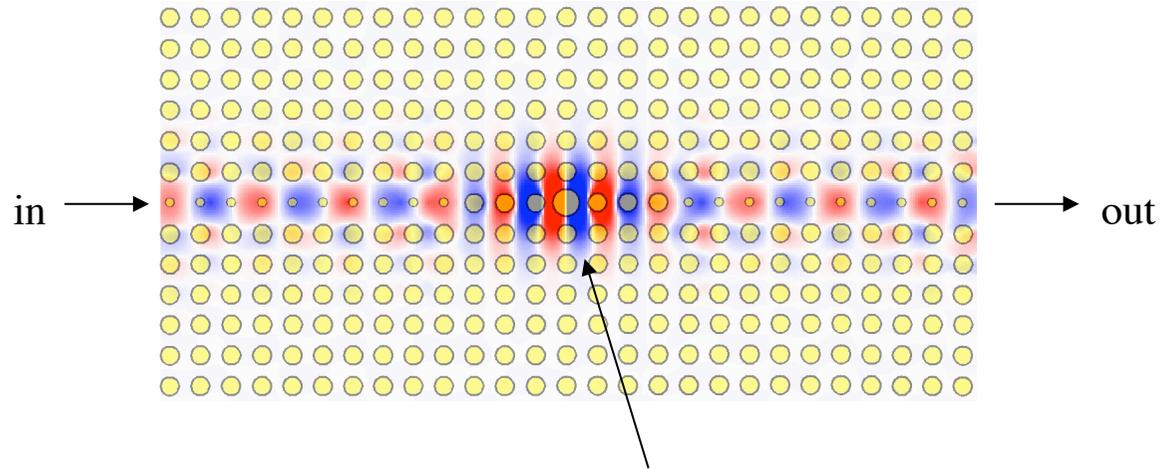
A Simple Linear Filter



Linear response:
Lorentzian Transmisson



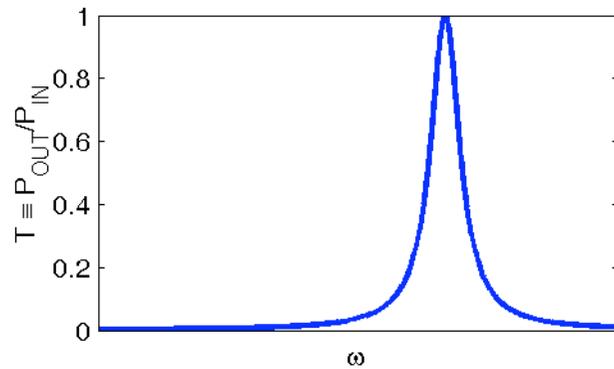
Filter + Kerr Nonlinearity?



Kerr nonlinearity:

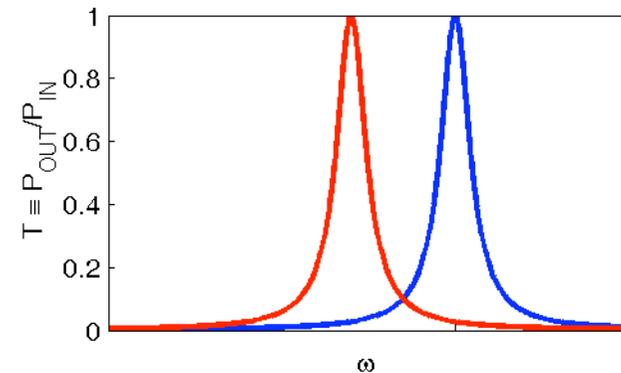
$$\Delta n \sim |E|^2$$

Linear response:
Lorentzian Transmisson



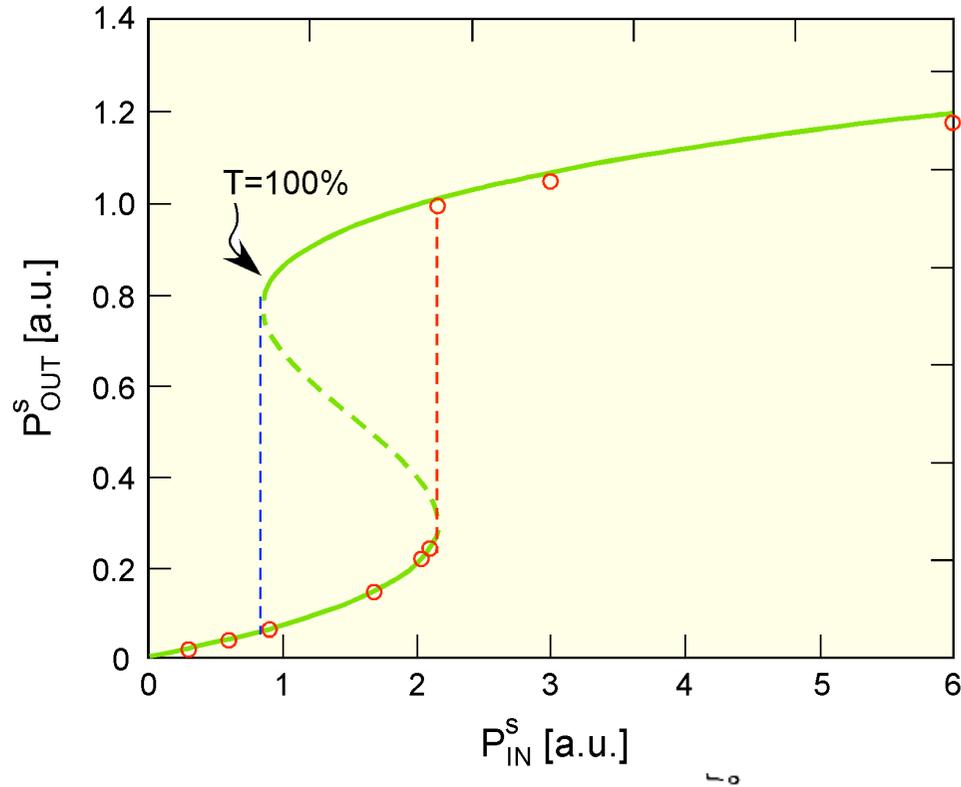
+ nonlinear
index shift
= ω shift

shifted peak?

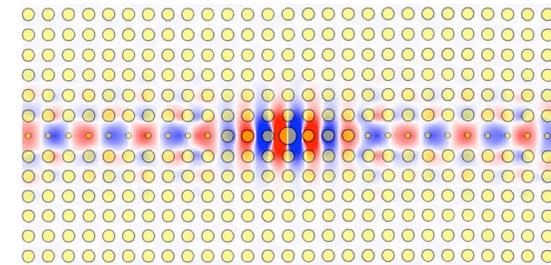


Optical Bistability

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



*Logic gates, switching,
rectifiers, amplifiers,
isolators, ...*



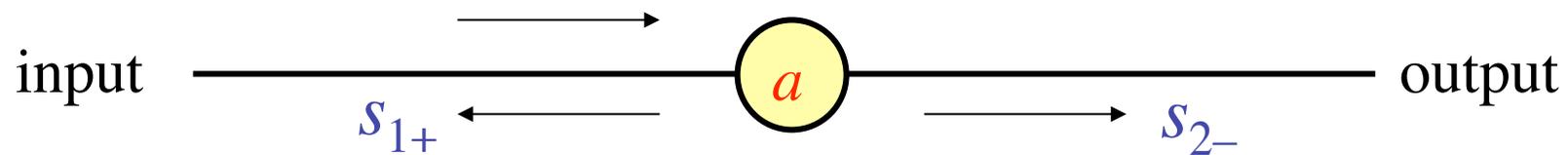
[Soljagic *et al.*,
PRE Rapid. Comm. **66**, 055601 (2002).]

Bistable (hysteresis) response
(& even multistable for multimode cavity)

Power threshold $\sim V/Q^2$
(in cavity with $V \sim (\lambda/2)^3$,
for Si and telecom bandwidth
power \sim 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)

$|s|^2 = \text{power}$

$|a|^2 = \text{energy}$

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

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

gives cubic equation
for transmission

... bistable curve

TCMT + Perturbation Theory

SPM = small change in refractive index

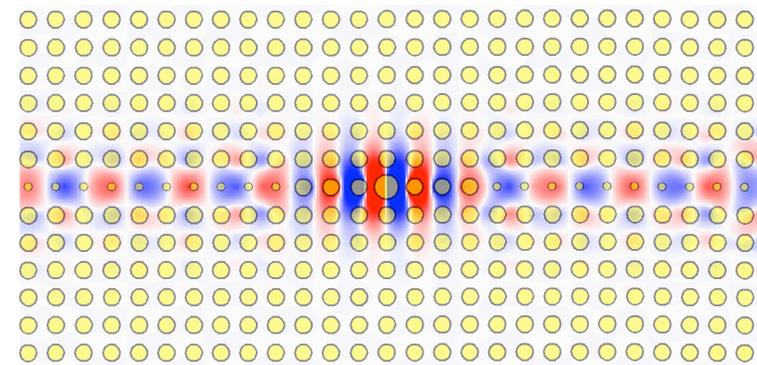
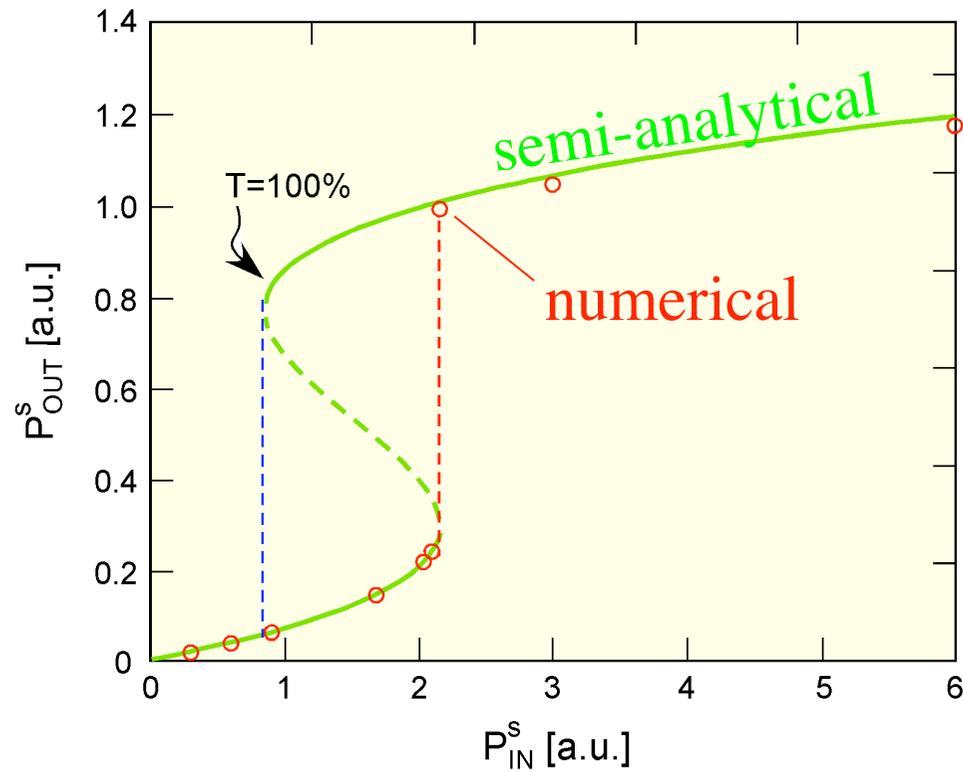
... evaluate $\Delta\omega$ by 1st-order perturbation theory

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

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

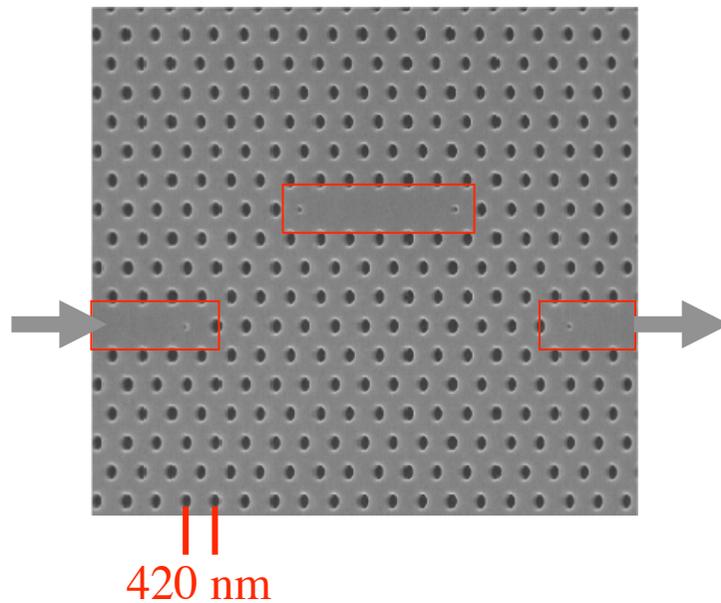
Accuracy of Coupled-Mode Theory

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



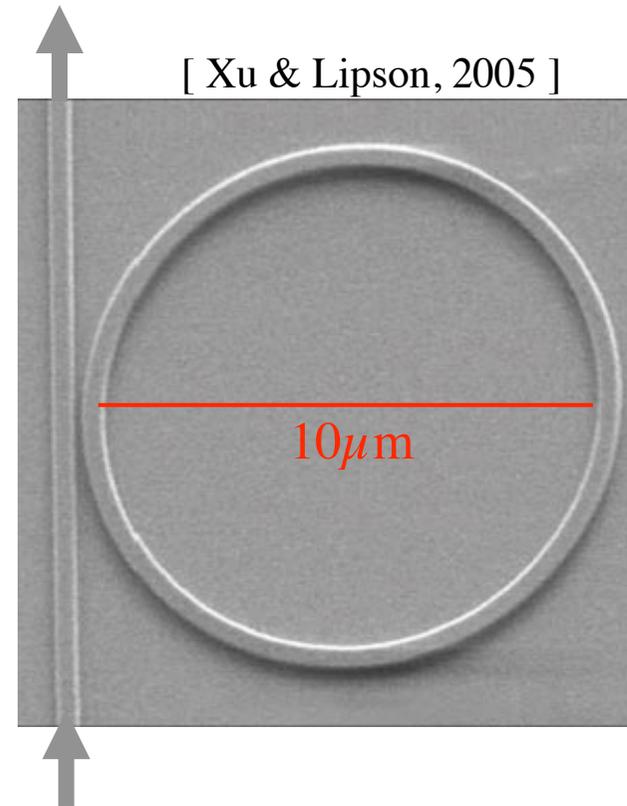
Optical Bistability in Practice

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



$Q \sim 30,000$
 $V \sim 10$ optimum
Power threshold $\sim 40 \mu\text{W}$

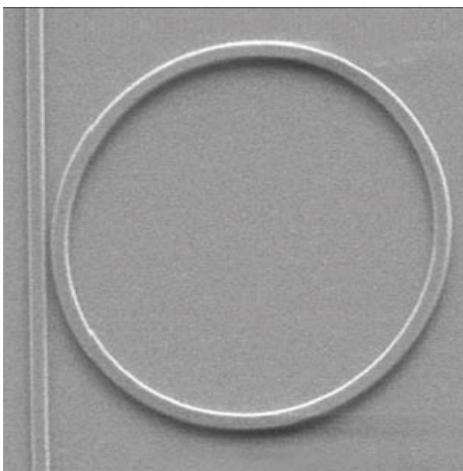
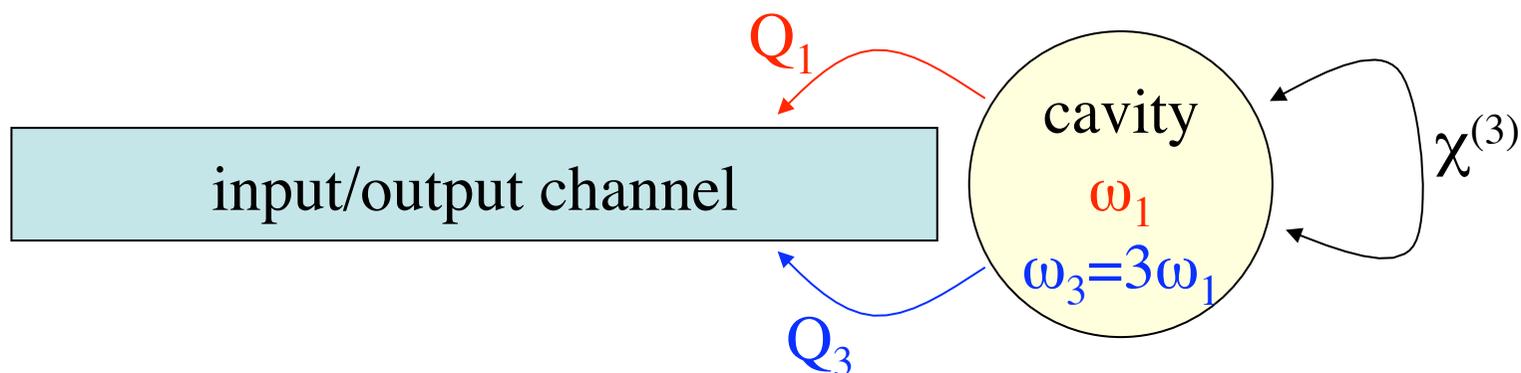
[Xu & Lipson, 2005]



$Q \sim 10,000$
 $V \sim 300$ optimum
Power threshold $\sim 10 \text{ mW}$

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

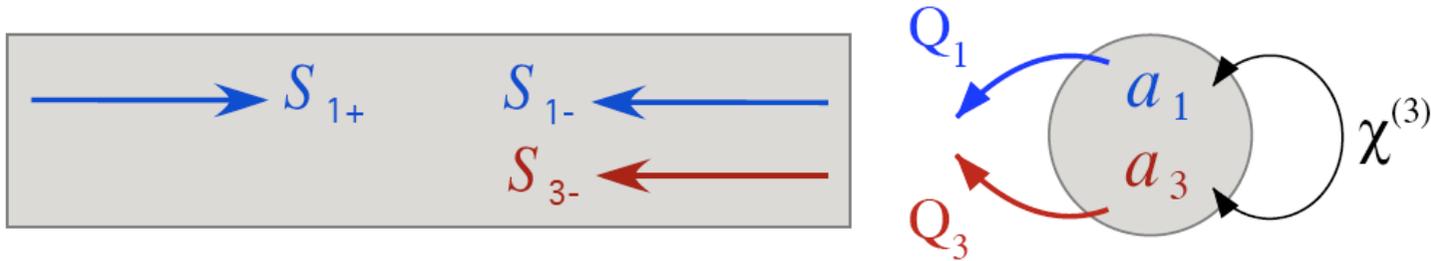
- must precisely tune ω_3 / ω_1
- materials must be ok at ω_1 and $3\omega_1$

But ... what if we could do it?

... what are the consequences?

Coupled-mode Theory for THG

third harmonic generation

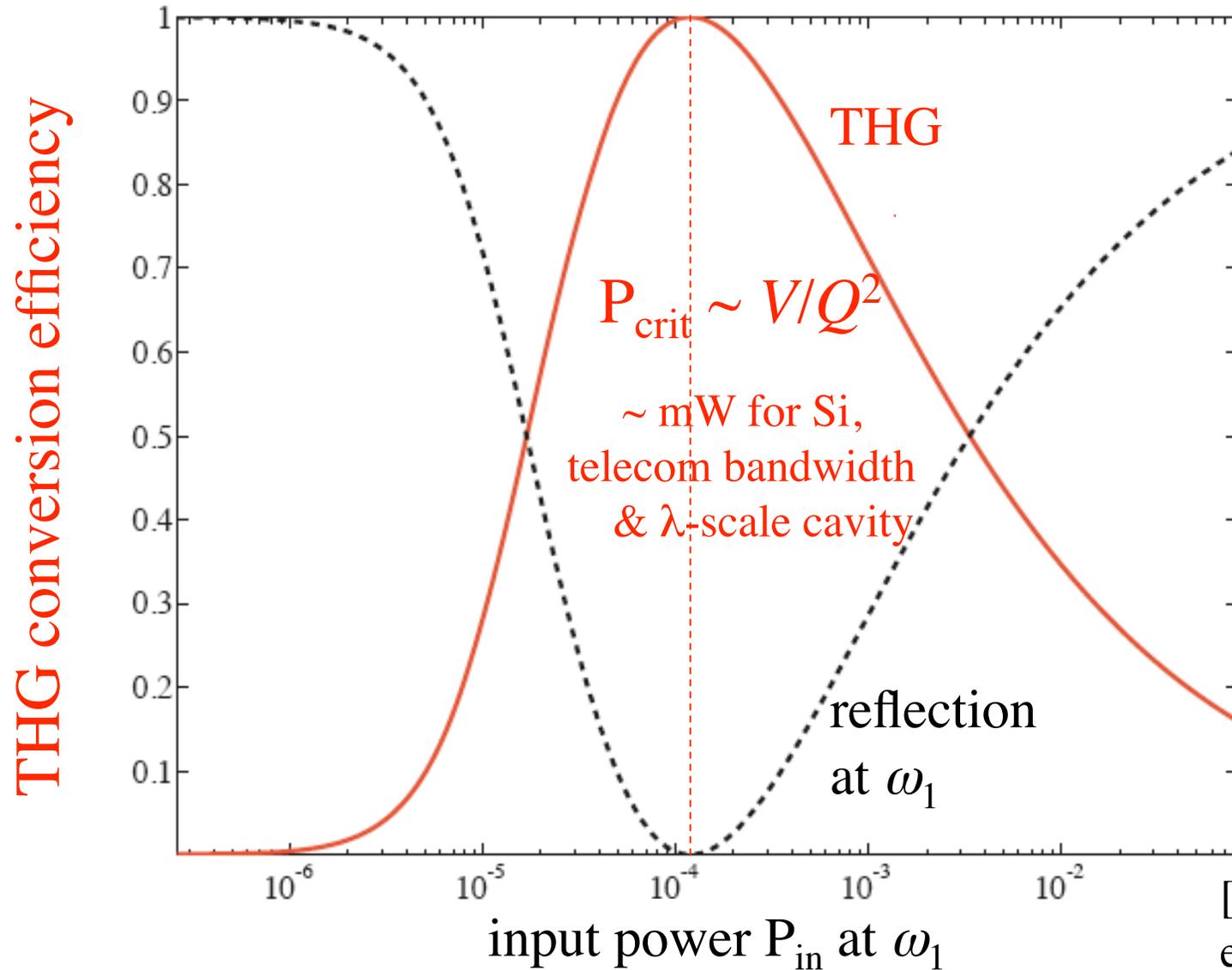


$$\begin{aligned}
 \frac{da_1}{dt} &= \left(\overset{\text{SPM}}{i\omega_1 (1 - \alpha_{11} |a_1|^2 - \alpha_{13} |a_3|^2)} - \frac{1}{\tau_1} \right) a_1 - \overset{\text{XPM}}{i\omega_1 \beta_1 (a_1^*)^2 a_3} + \overset{\text{down-conversion}}{\sqrt{\frac{2}{\tau_{s,1}}} s_+} \\
 \frac{da_3}{dt} &= \left(\overset{\text{SPM}}{i\omega_3 (1 - \alpha_{33} |a_3|^2 - \alpha_{31} |a_1|^2)} - \frac{1}{\tau_3} \right) a_3 - \overset{\text{THG}}{i\omega_3 \beta_3 a_1^3} + \sqrt{\frac{2}{\tau_{s,3}}} s_+
 \end{aligned}$$

[Rodriguez et al. (2007)]

$\alpha=0$: Critical Power for Efficient THG

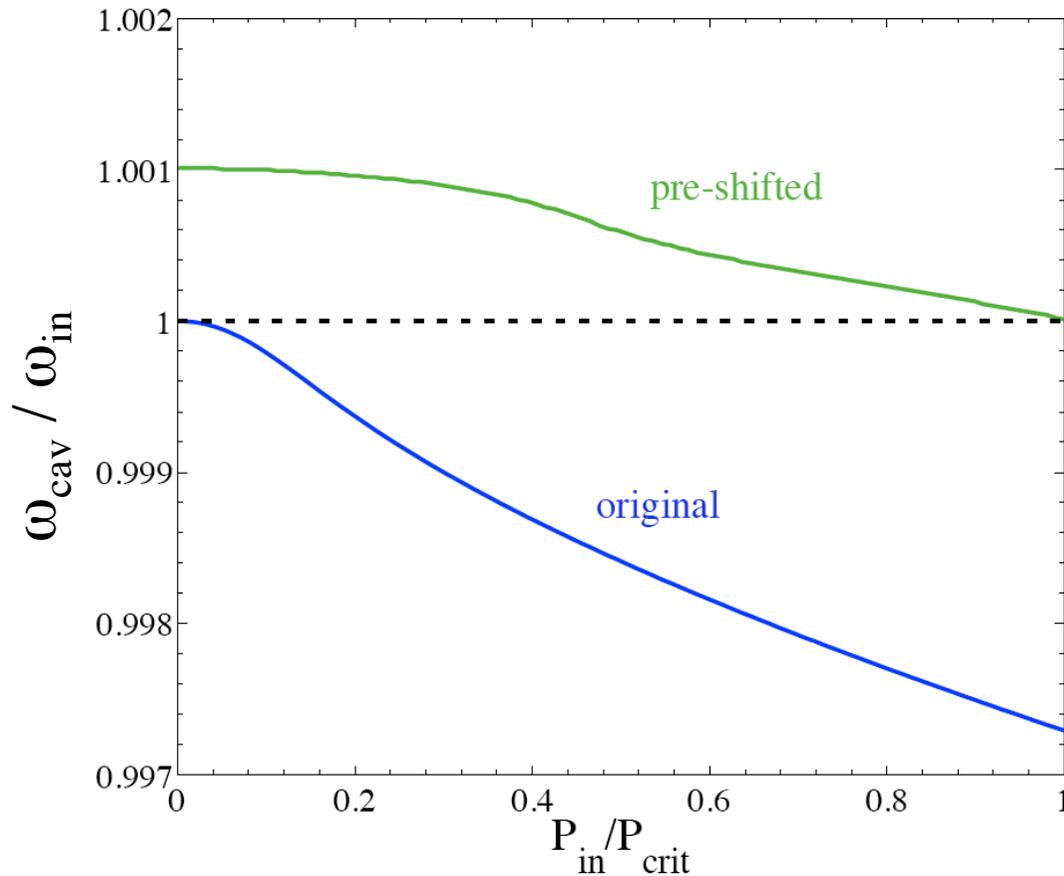
third-harmonic generation in doubly-resonant $\chi^{(3)}$ (Kerr) cavity



[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?

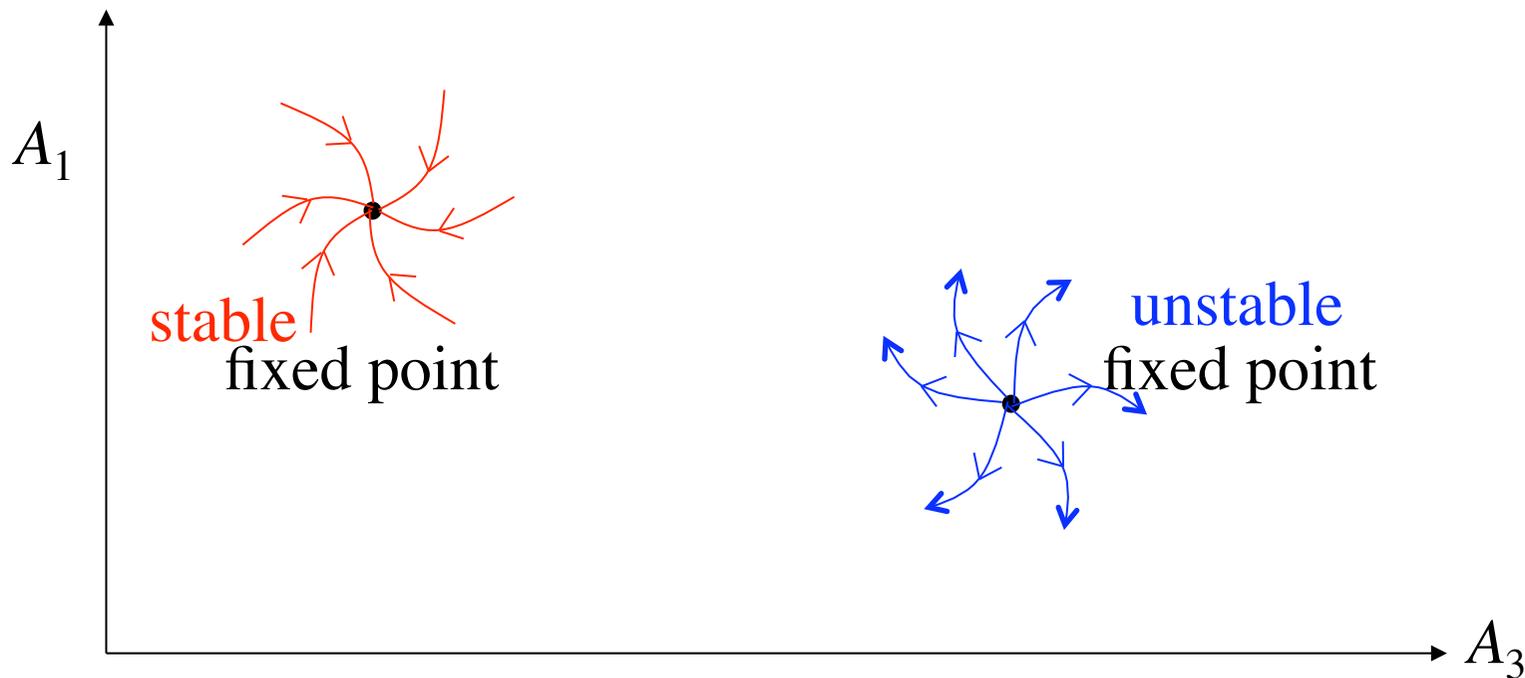
brief review

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**



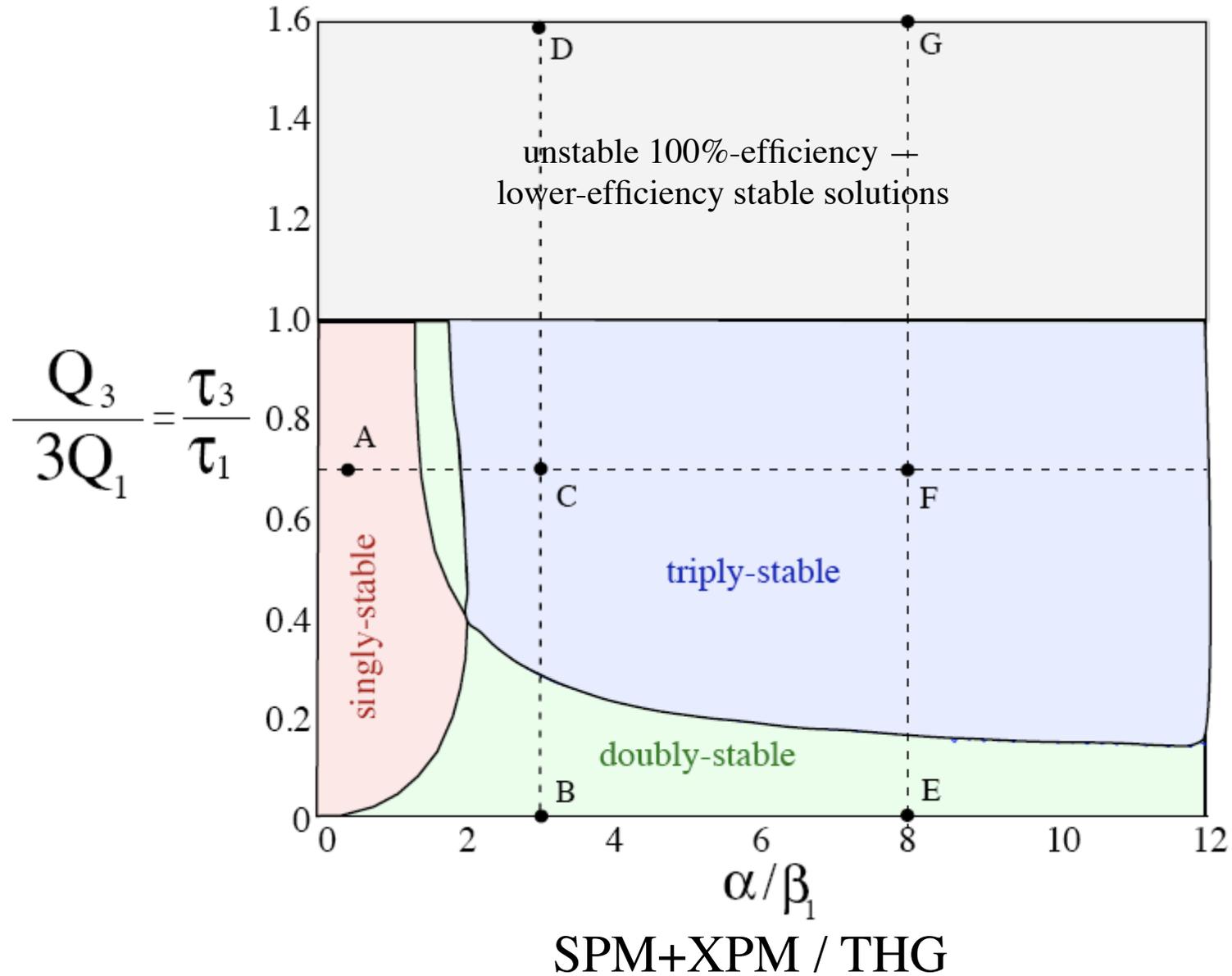
cartoon phase space (A_1, A_3 are actually complex)

for simplicity, assume SPM = XPM coefficients:

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

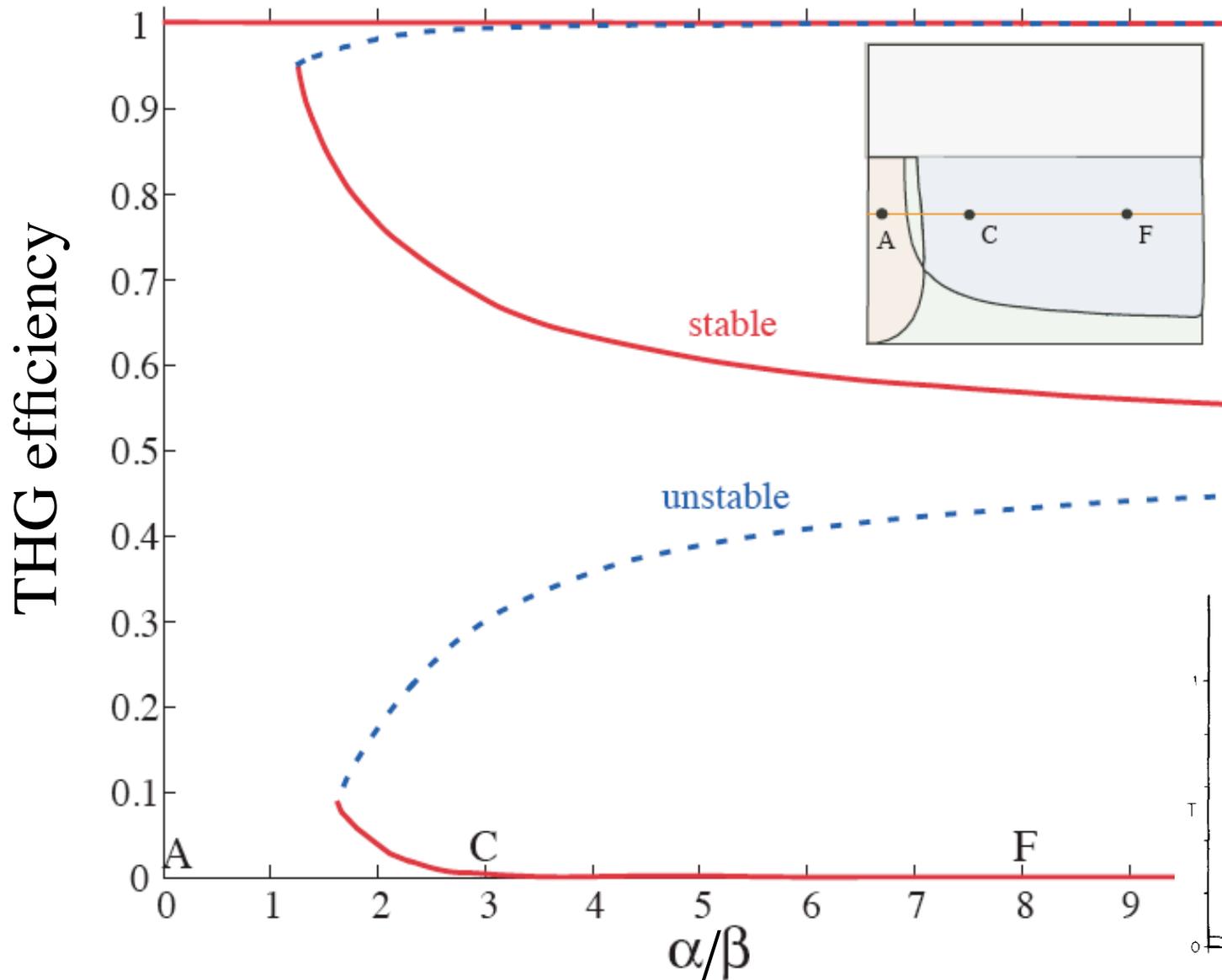
THG Stability Phase Diagram

[Hashemi et al (2008)]

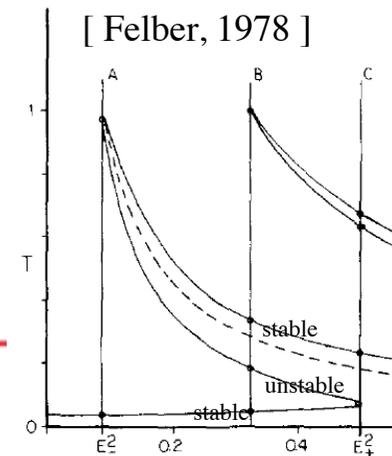


Bifurcation vs. SPM/XPM

[Hashemi et al (2008)]



[Felber, 1978]



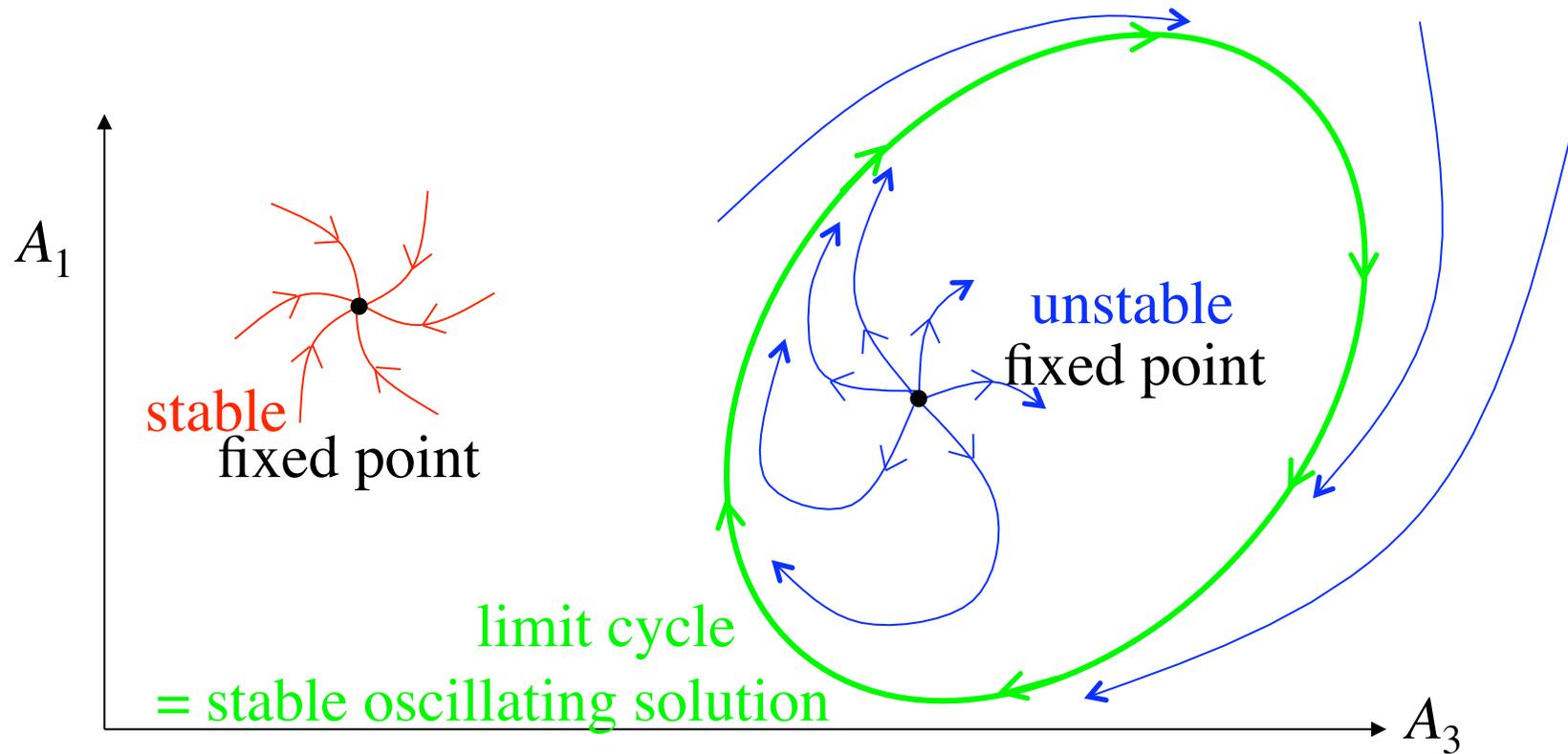
Limit Cycles

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

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

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

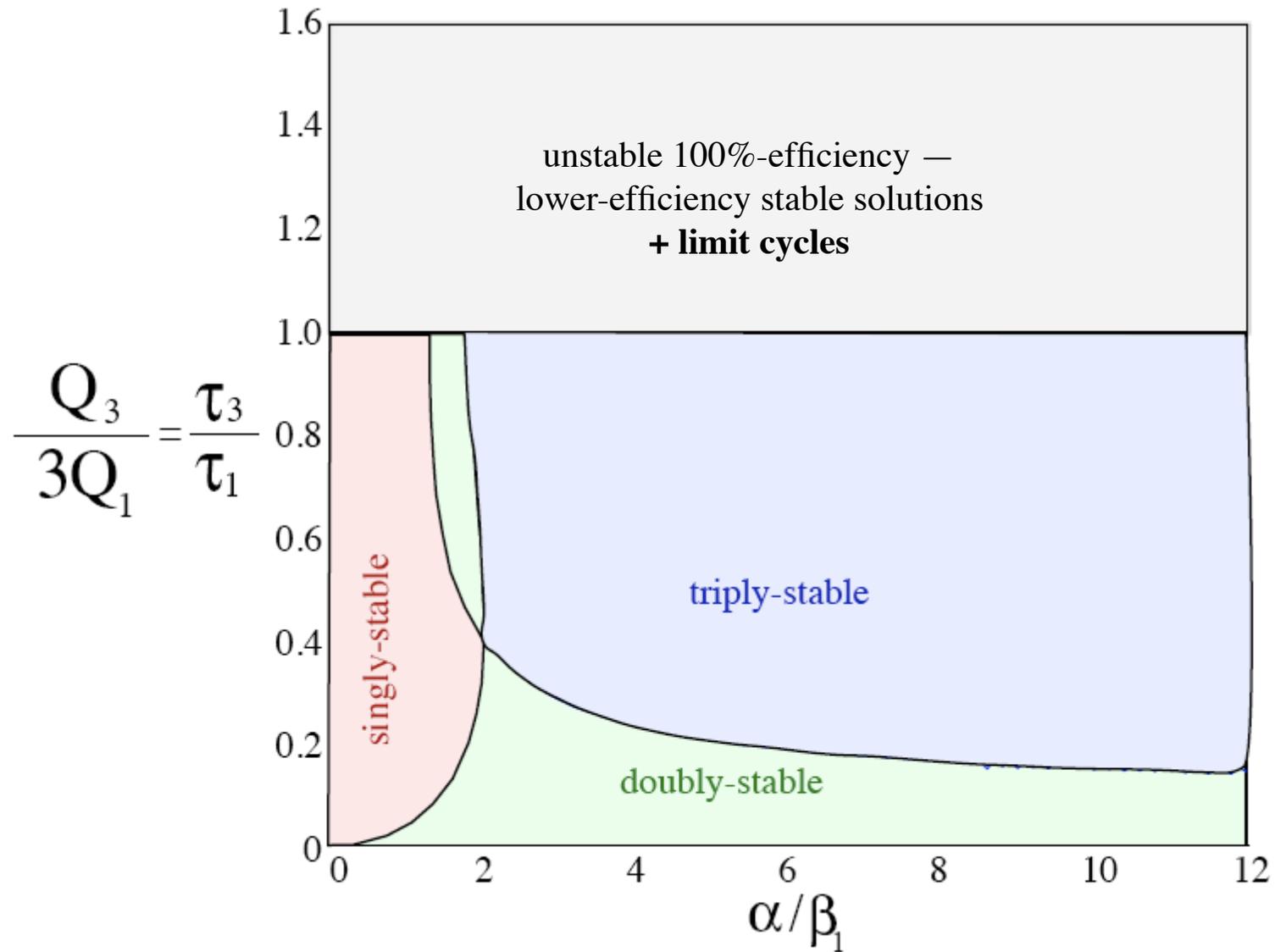
then steady state = A_1, A_3 constant = **fixed-point**



cartoon phase space (A_1, A_3 are actually complex)

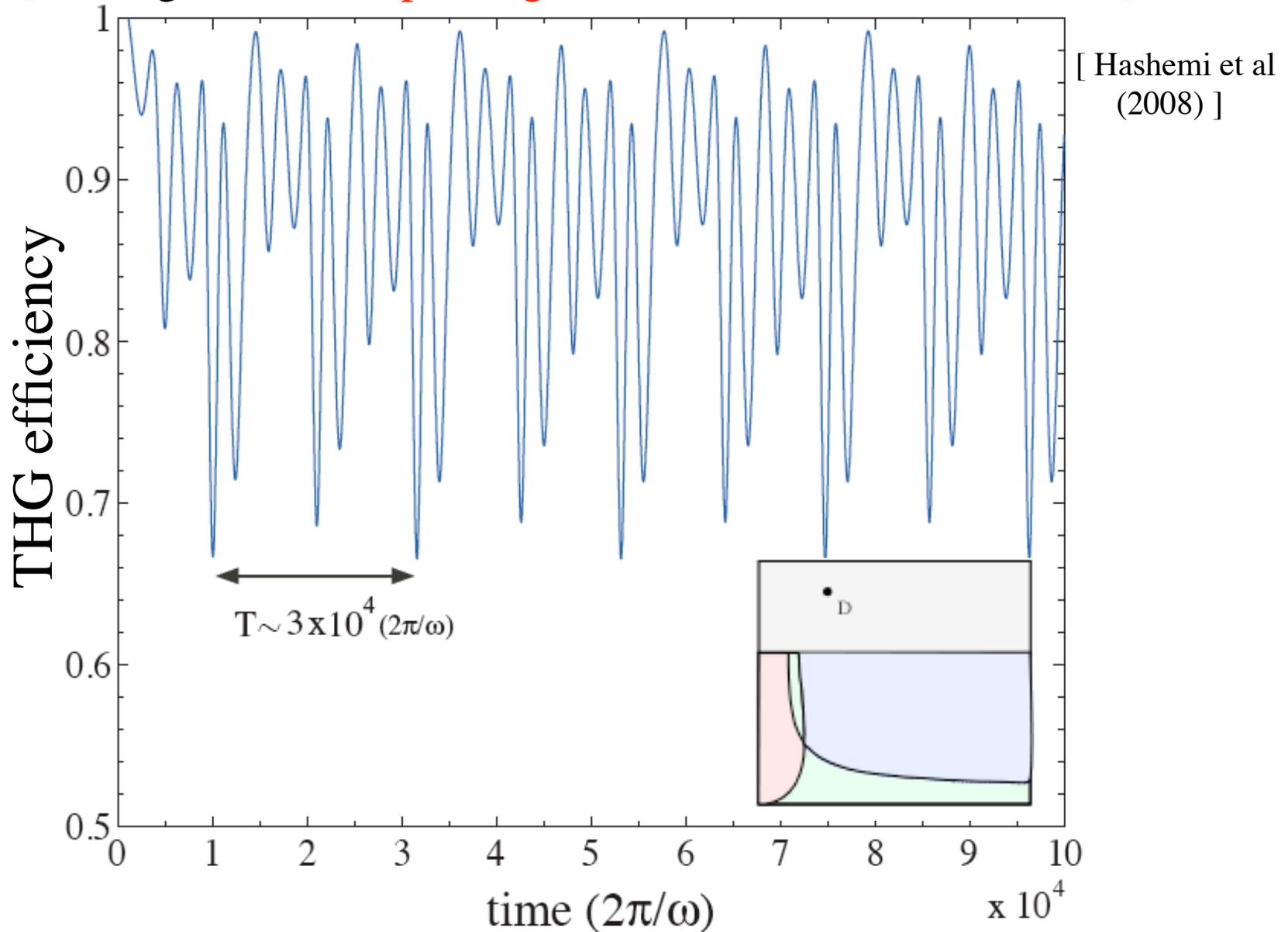
Stability Phase Diagram

[Hashemi et al (2008)]



An Optical Kerr-THG Oscillator

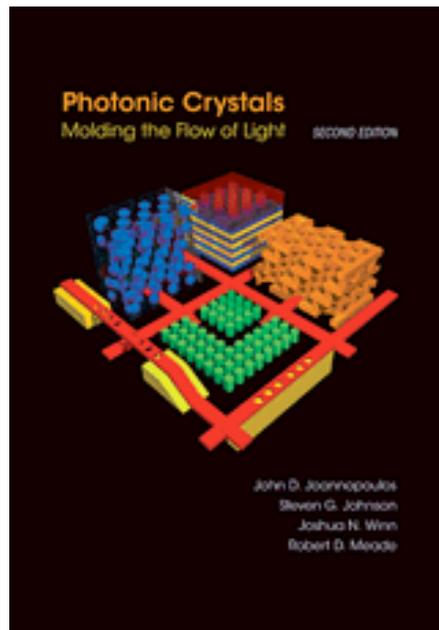
[analogous to **self-pulsing** in SHG; Drummond (1980)]



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://jdg.mit.edu/book>
(covers coupled-mode theory etc.)

Free FDTD software: <http://jdg.mit.edu/meep>
& tutorials

PML notes:

<http://math.mit.edu/~stevenj/18.369/pml.pdf>