



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



**2145-22**

**Spring College on Computational Nanoscience**

*17 - 28 May 2010*

**Computational Photonics: Cavities and Resonant Devices**

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USA*

# Computational Nanophotonics: Cavities and Resonant Devices

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MIT Applied Mathematics

# Resonance

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

frequency  $\omega_0$

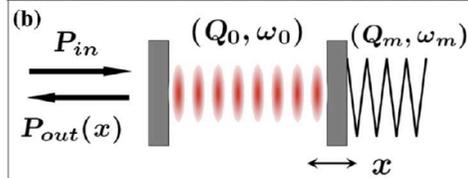
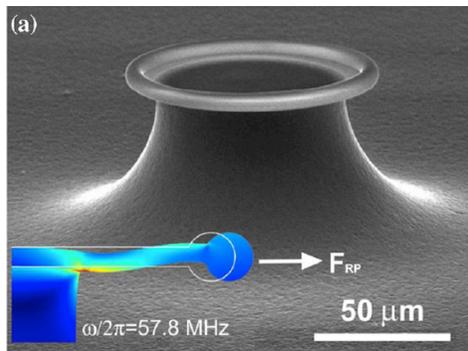
lifetime  $\tau \gg 2\pi/\omega_0$

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

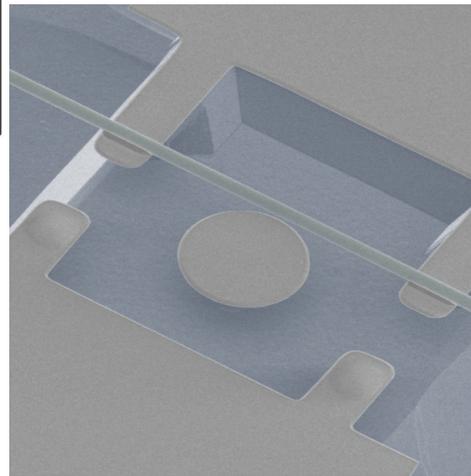
modal  
volume  $V$

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

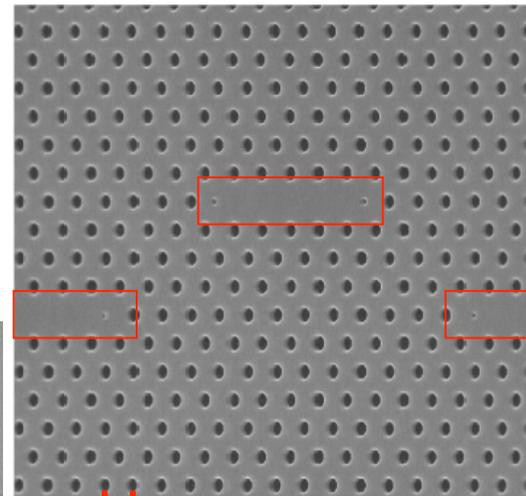
[ Notomi *et al.* (2005). ]



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

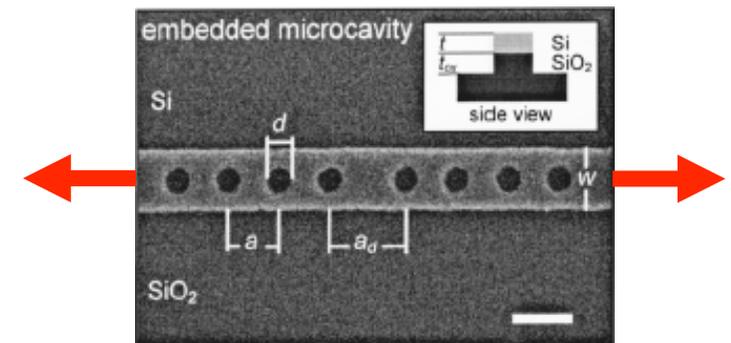


[ Eichenfield *et al.* *Nature Photonics* **1**, 416 (2007) ]



420 nm

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



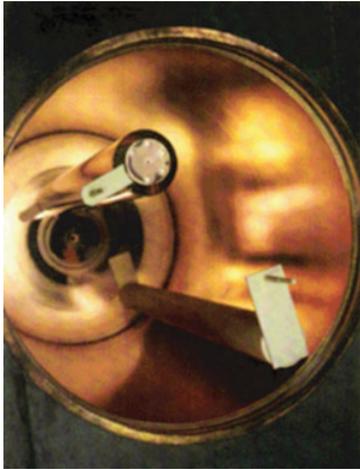
# Why Resonance?

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, ...

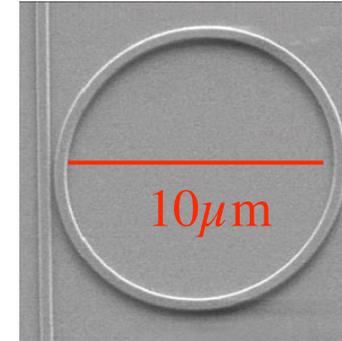
# How Resonance?

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



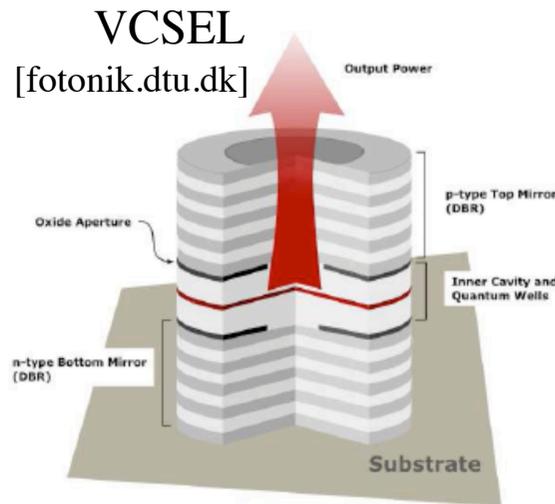
[ llnl.gov ]

**metallic cavities:**  
good for microwave,  
**dissipative** for infrared



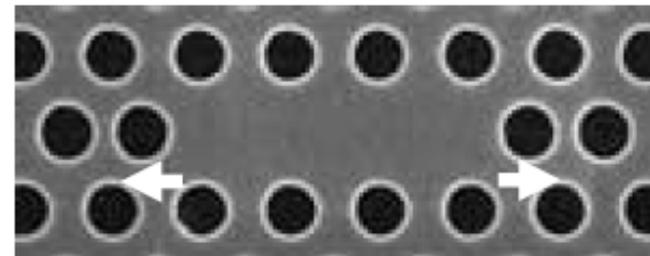
[ Xu & Lipson (2005) ]

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

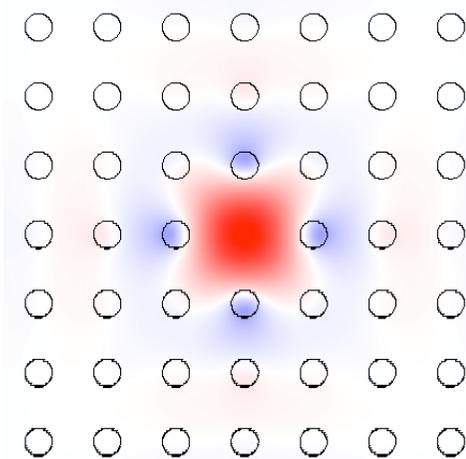


**photonic bandgaps**  
(complete or partial  
+ index-guiding)

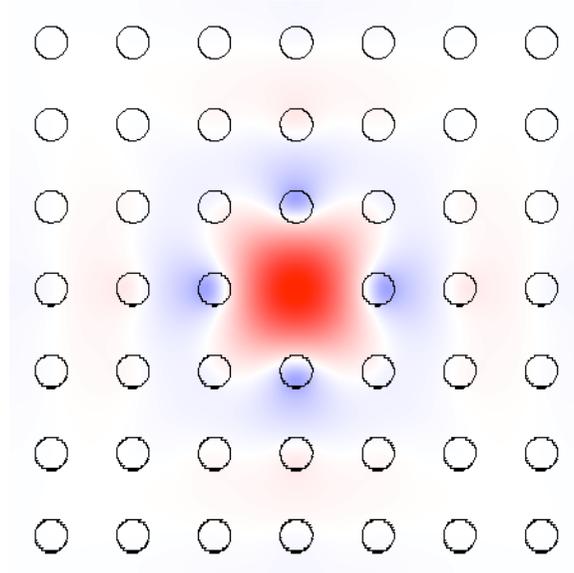
[ Akahane, *Nature* **425**, 944 (2003) ]



(planar Si slab)



# Microcavity Blues

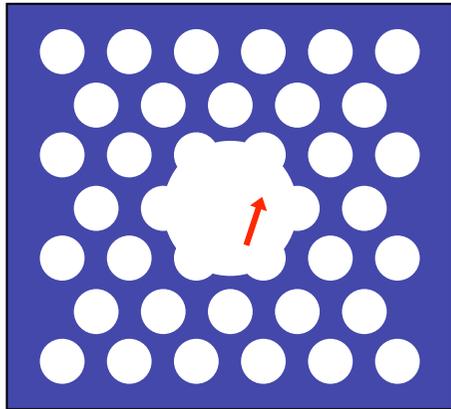


For cavities (*point defects*)  
frequency-domain has its drawbacks:

- Best methods compute lowest- $\omega$  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*

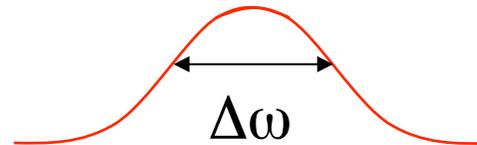
# Time-Domain Eigensolvers

(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*

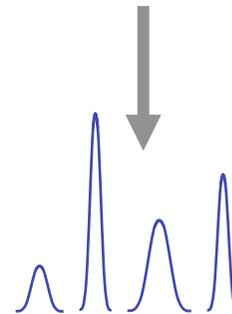
*signal processing*

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

**complex**  $\omega_n$



decay rate in time gives **loss**



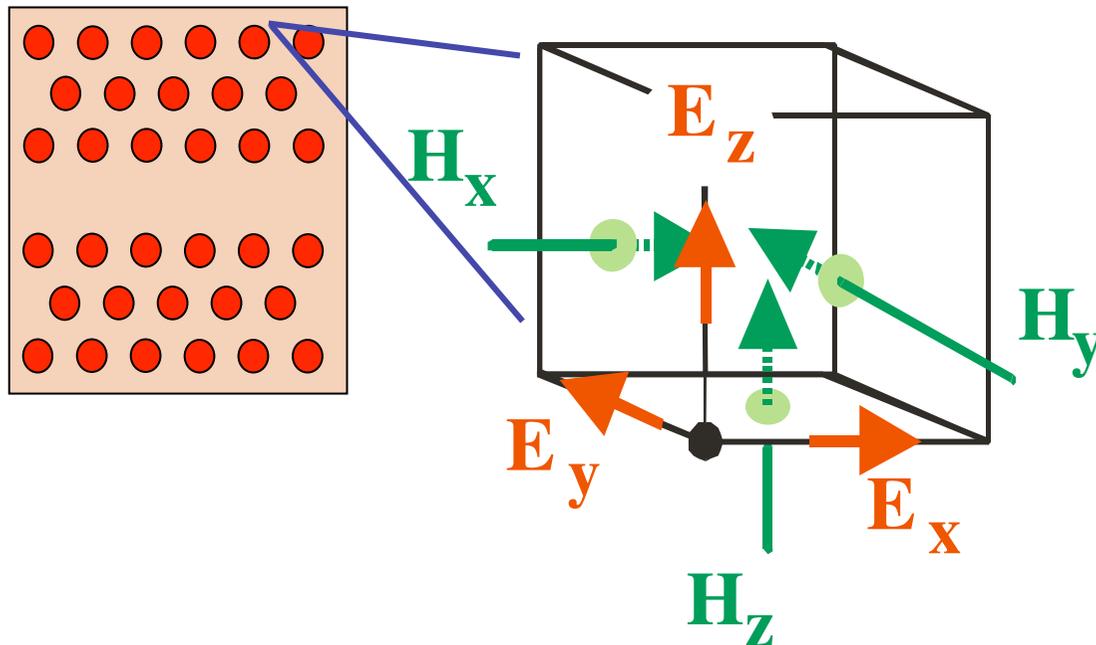
Response is many  
sharp peaks,  
**one peak per mode**

# 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

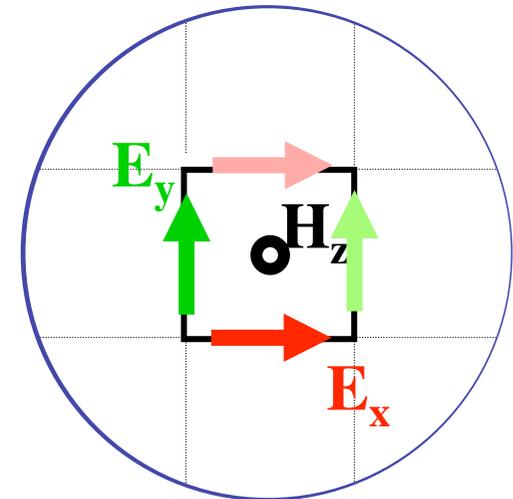
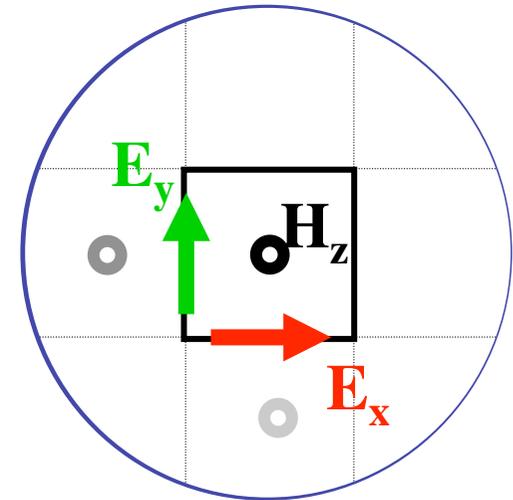
using spatial derivatives of  $\mathbf{H}$ , then find  $\mathbf{E} = \epsilon^{-1} \mathbf{D}$  ( $\epsilon$  constant)

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

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

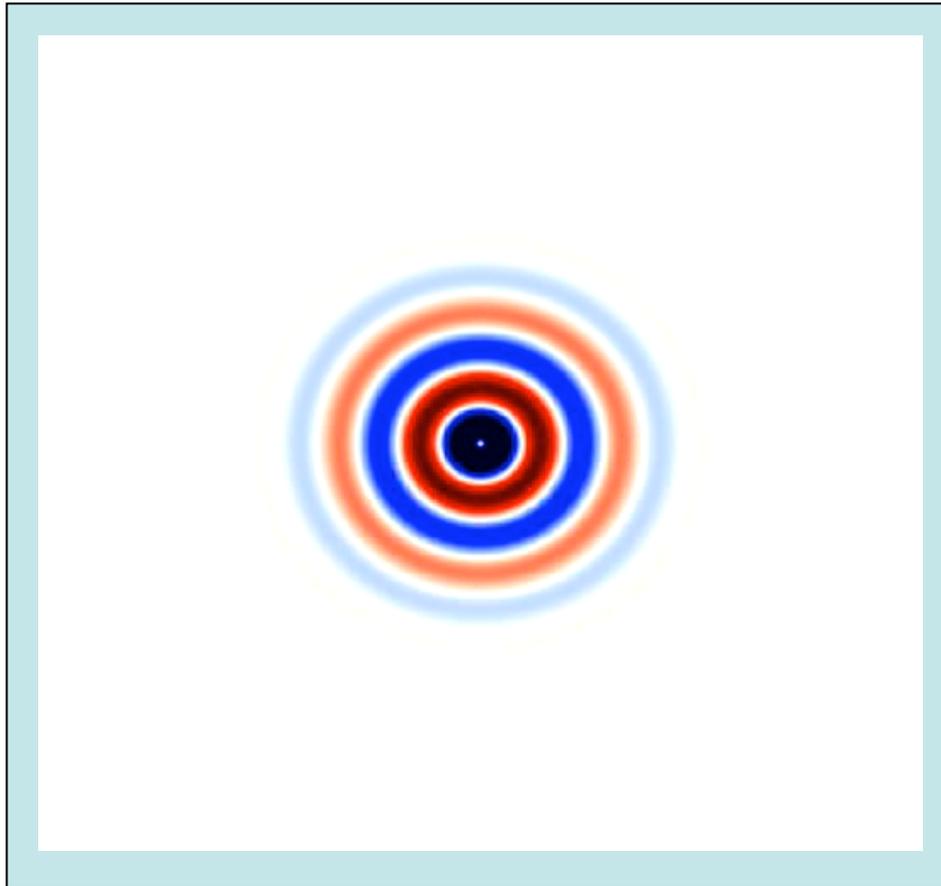
2) at time  $t+0.5$ : Update  $\mathbf{H}$  fields everywhere using spatial derivatives of  $\mathbf{E}$  ( $\mu$  constant)

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



# Why Absorbers?

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



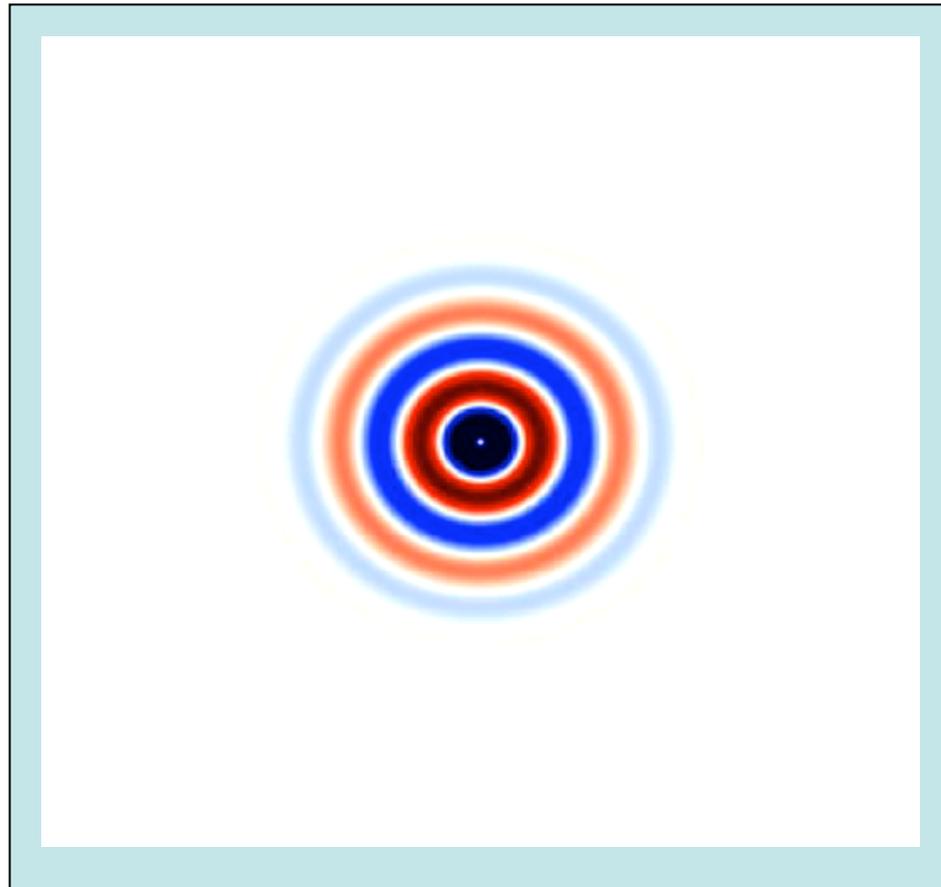
In a wave equation, a hard-wall **truncation** gives **reflection artifacts**.

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.

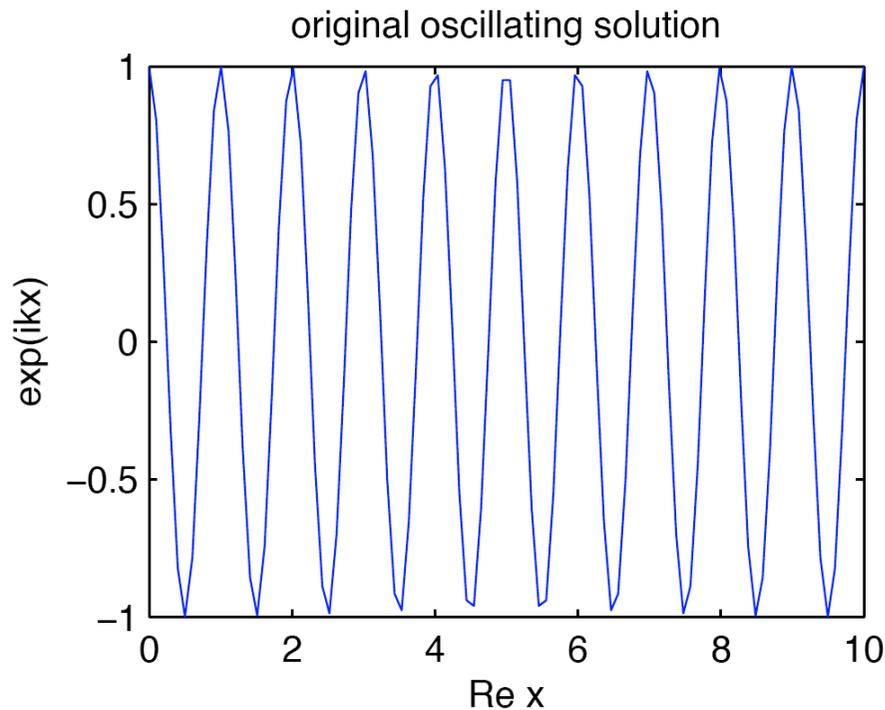
Several derivations, cleanest  
& most general via “**complex  
coordinate stretching**”

[ 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  $\omega > 0$ .

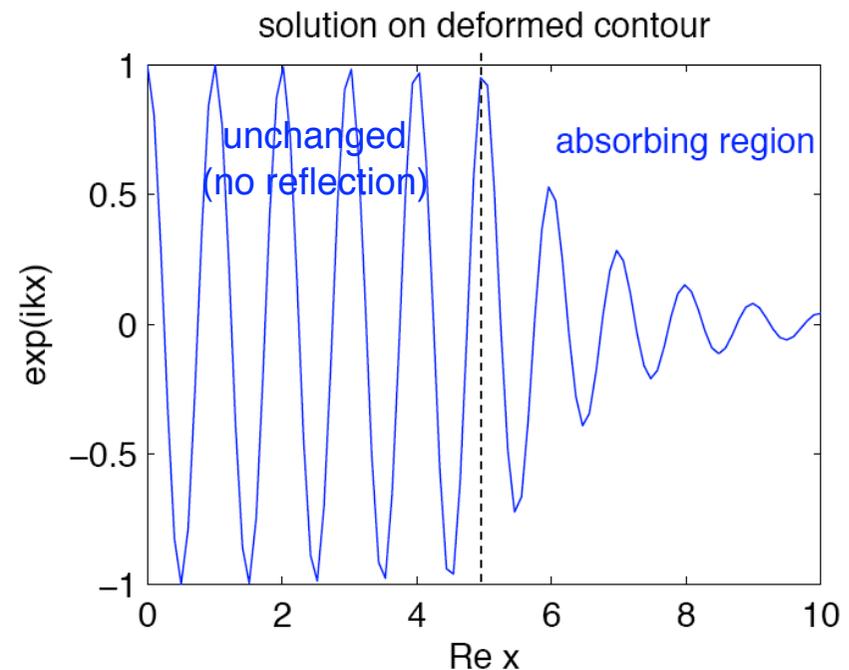
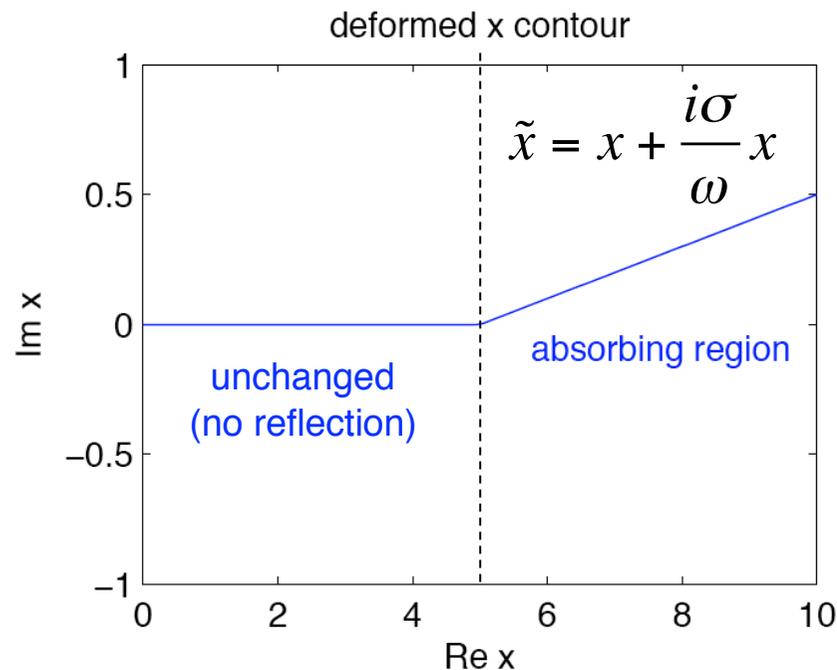
$$\text{fields} \sim f(y, z) e^{i(kx - \omega t)} \quad (\text{usually, } k > 0)$$



(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  $\sigma$ )

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

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

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

# PML Step 3: Effective materials

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

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

$x$  PML Jacobian

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

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

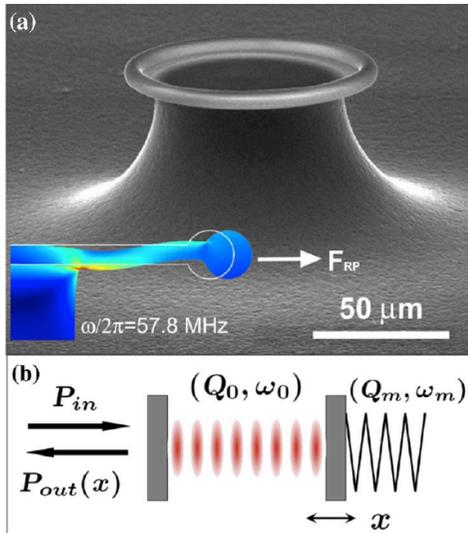
for isotropic starting materials:

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

effective conductivity

PML = effective anisotropic “absorbing”  $\epsilon, \mu$

# 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**

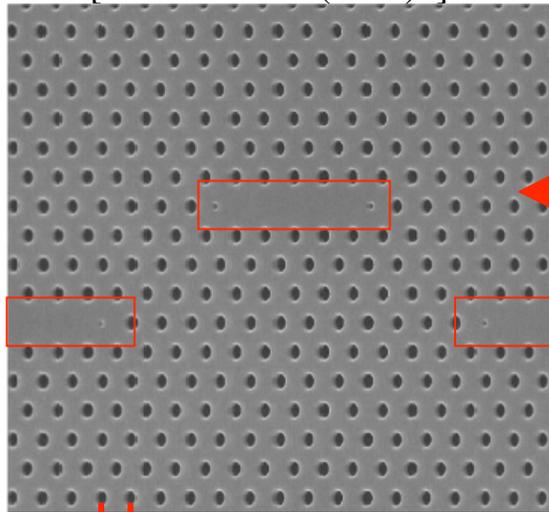
# “Temporal coupled-mode theory”

- 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](http://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)

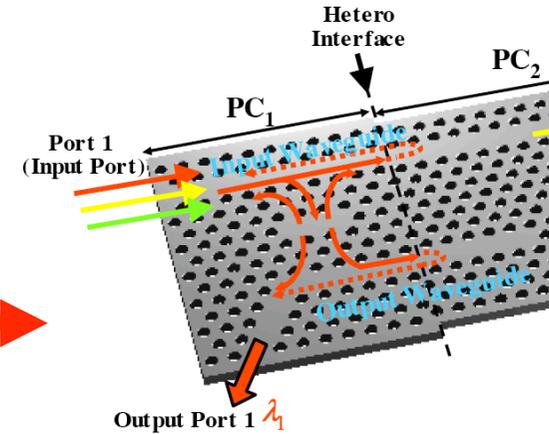
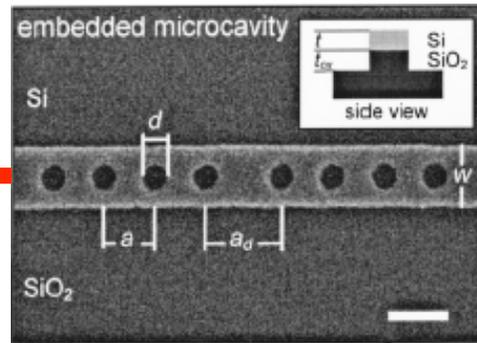
# TCMT example: a linear filter

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

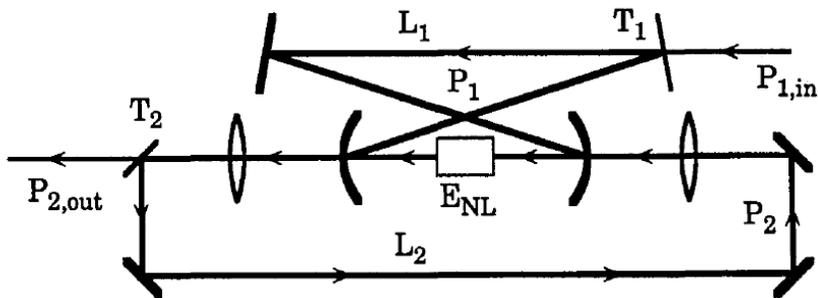


420 nm

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



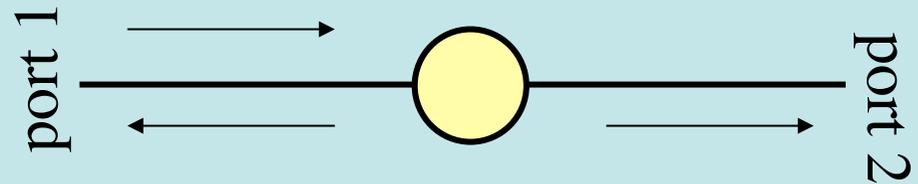
[ Takano *et al.* (2006) ]



[ Ou & Kimble (1993) ]

= abstractly:

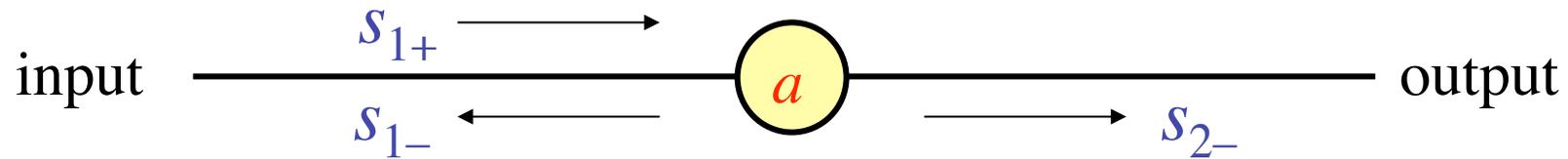
two single-mode i/o ports  
+ one resonance



resonant cavity  
frequency  $\omega_0$ , lifetime  $\tau$

# Temporal Coupled-Mode Theory

for a linear filter



resonant cavity

frequency  $\omega_0$ , lifetime  $\tau$

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

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

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

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

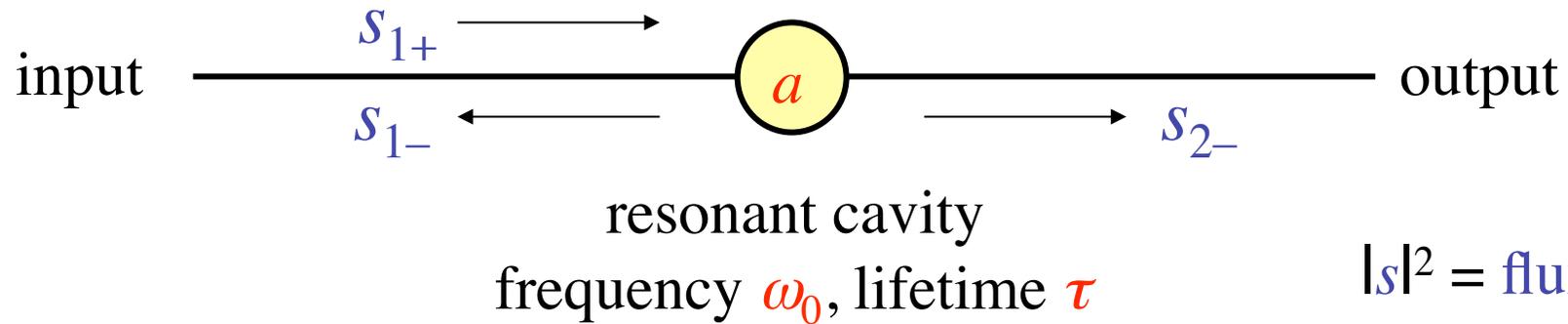
*can be relaxed*

assumes only:

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

# Temporal Coupled-Mode Theory

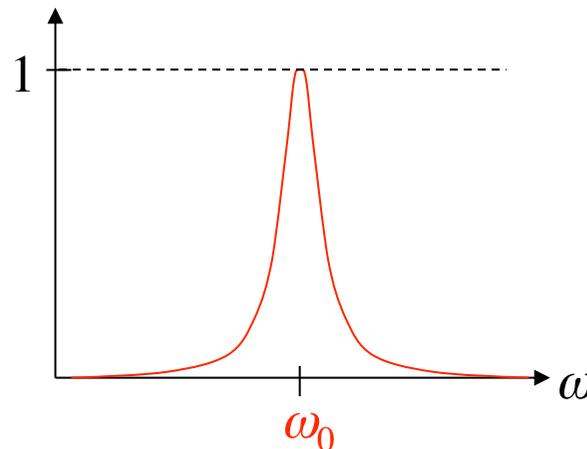
for a linear filter



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

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

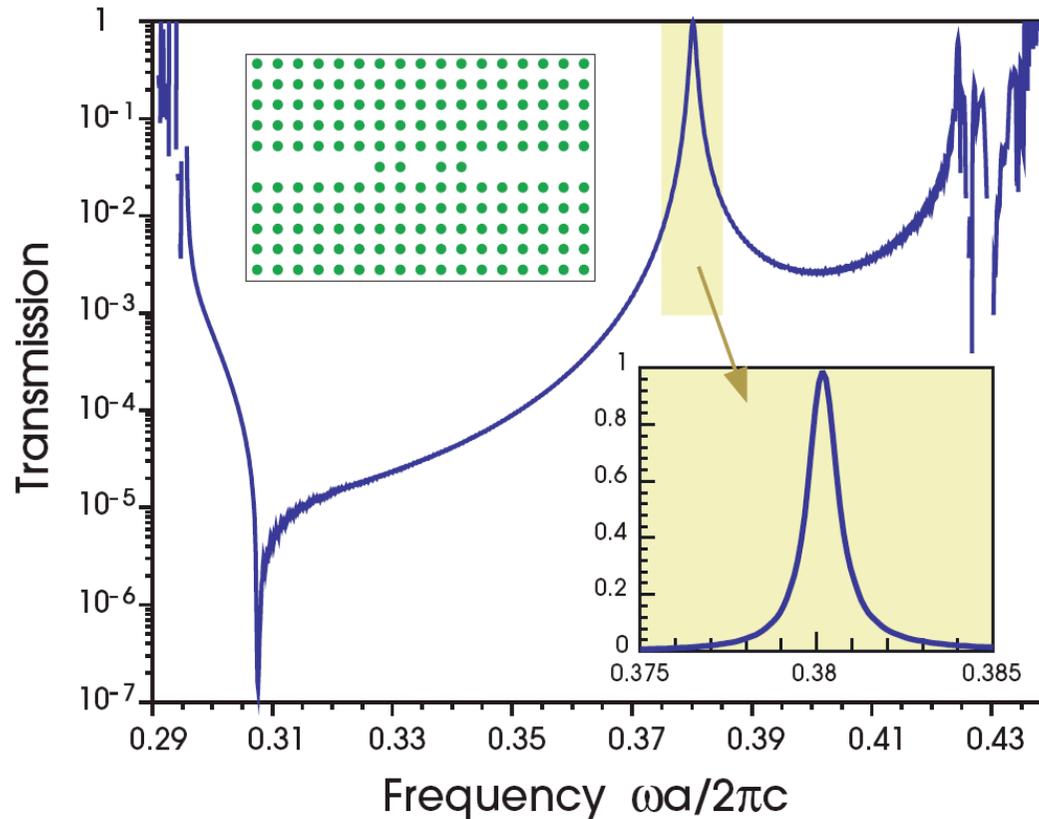
transmission  $T$   
 $= |s_{2-}|^2 / |s_{1+}|^2$



$T =$  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**

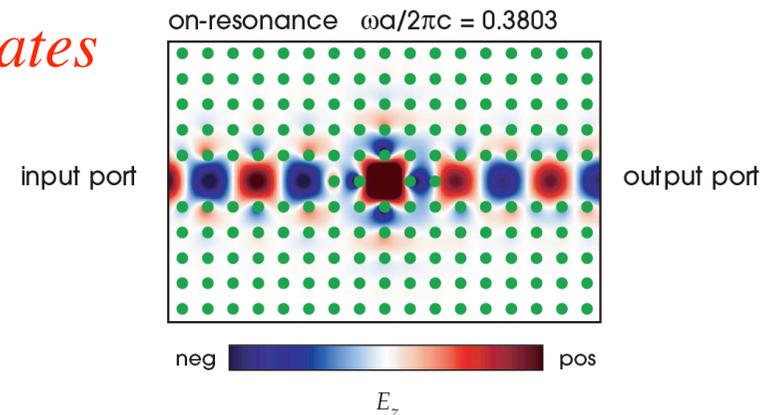
cavity **decays to input/output with equal rates**

⇒ At resonance, **reflected** wave

**destructively interferes**

with **backwards-decay** from cavity

& the two **exactly cancel**.



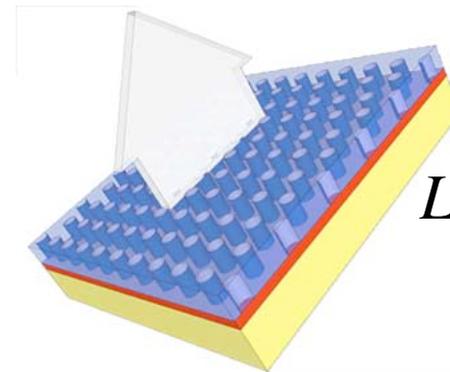
# Some interesting resonant transmission processes



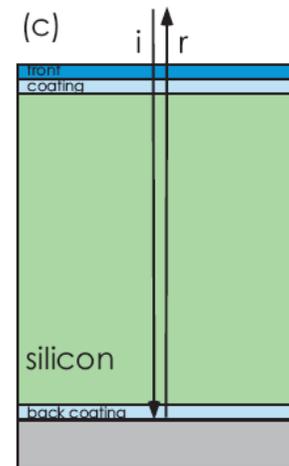
Wireless resonant power transfer

[ M. Soljacic, MIT (2007) ]

witricity.com



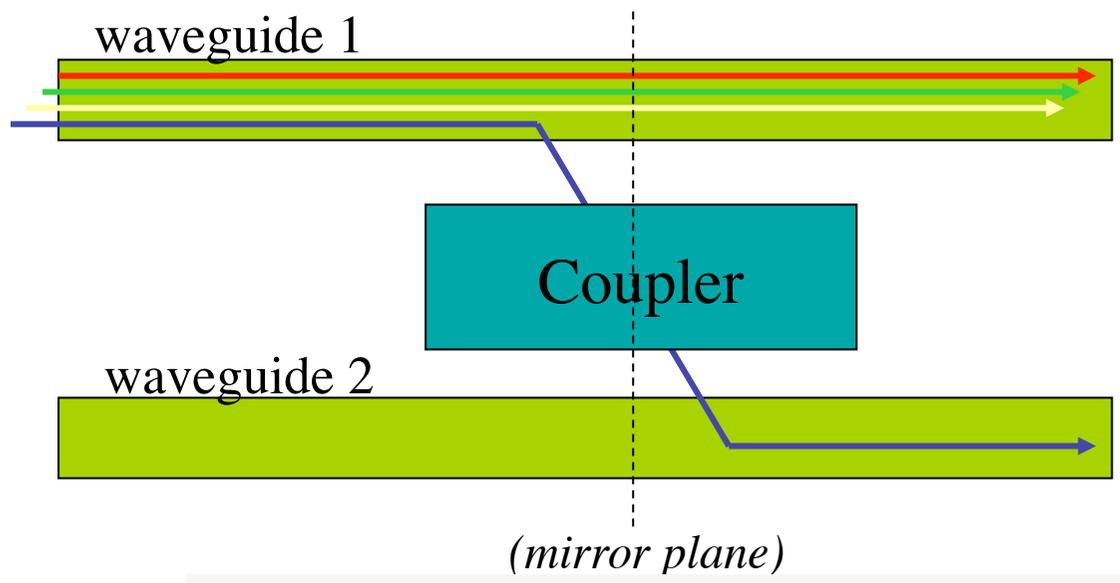
*Resonant  
LED emission*  
luminus.com



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

[ e.g. Ghebrebrhan (2009) ]

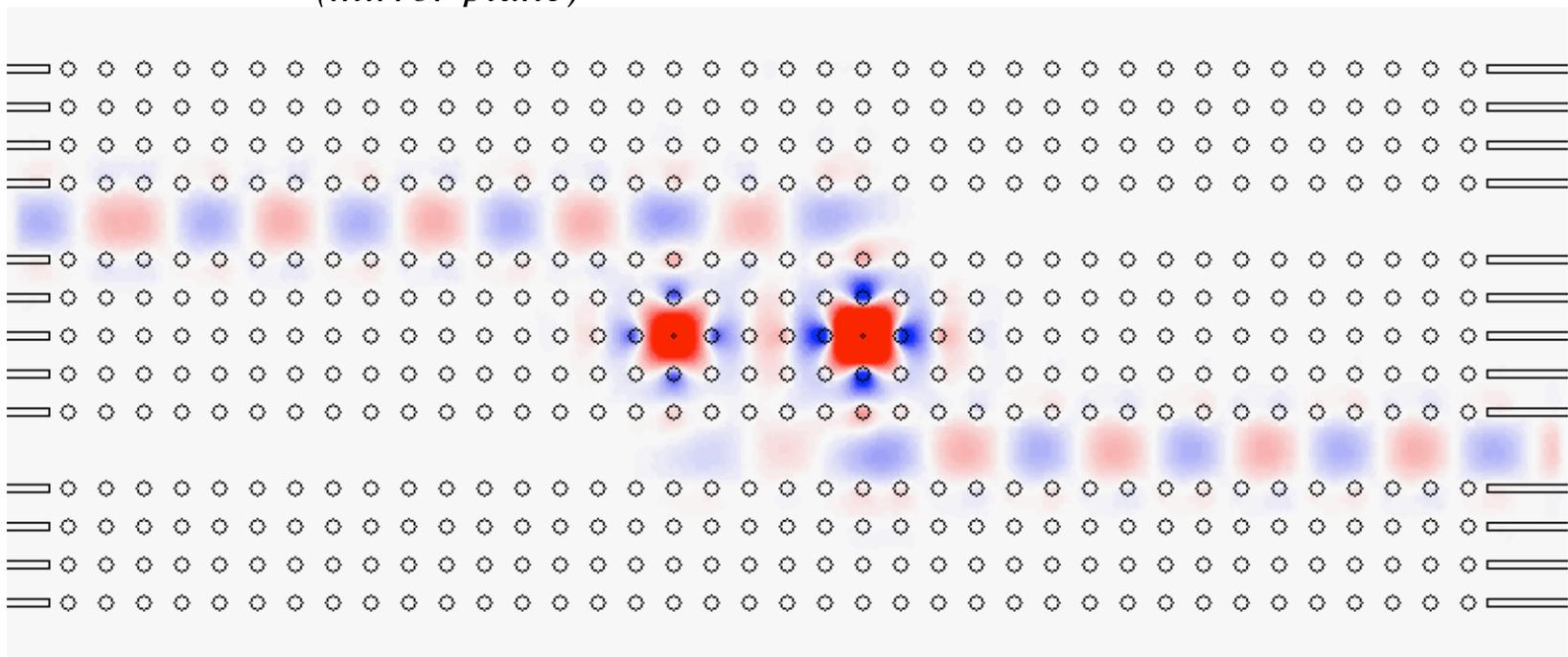
# Another interesting example: Channel-Drop Filters



*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: $Q$

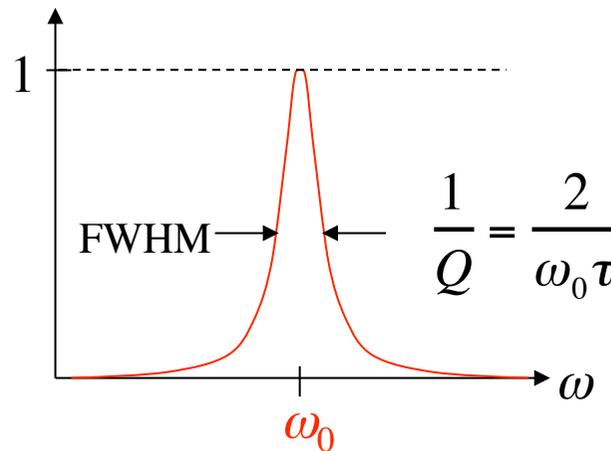
$$Q = \omega_0 \tau / 2$$

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:*



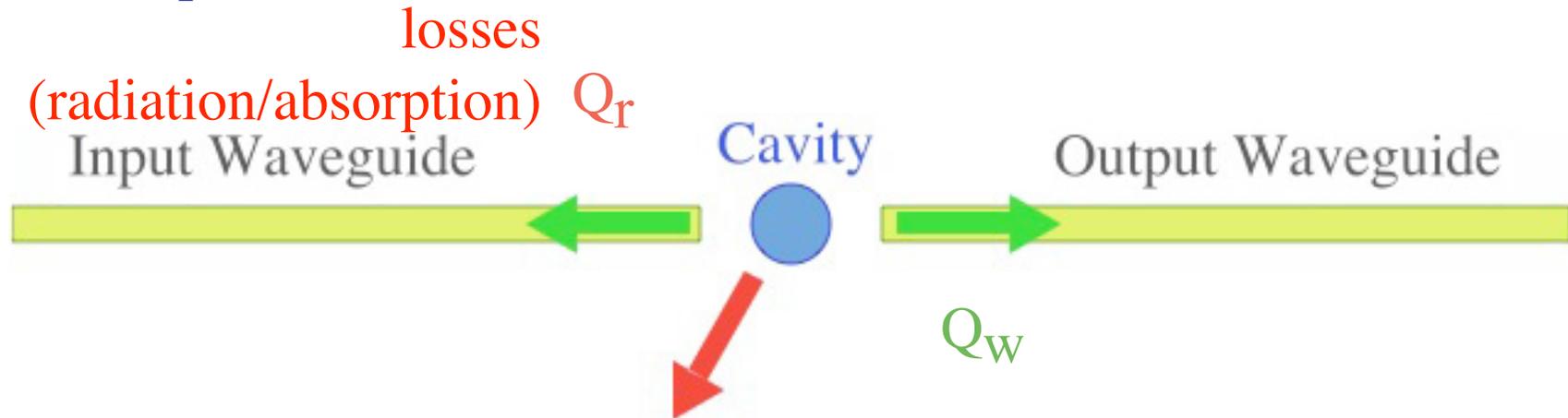
$T = \text{Lorentzian filter}$

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

...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!*

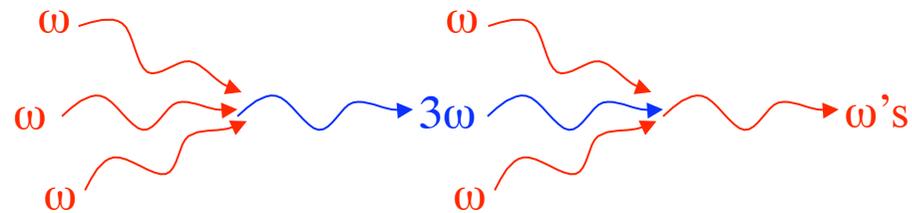
nonlinearities + microcavities

= *qualitatively* new phenomena

# Nonlinear Optics

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

- Self-Phase Modulation (**SPM**)  
= change in refractive index( $\omega$ )  $\sim |\mathbf{E}(\omega)|^2$
- Cross-Phase Modulation (**XPM**)  
= change in refractive index( $\omega$ )  $\sim |\mathbf{E}(\omega_2)|^2$
- 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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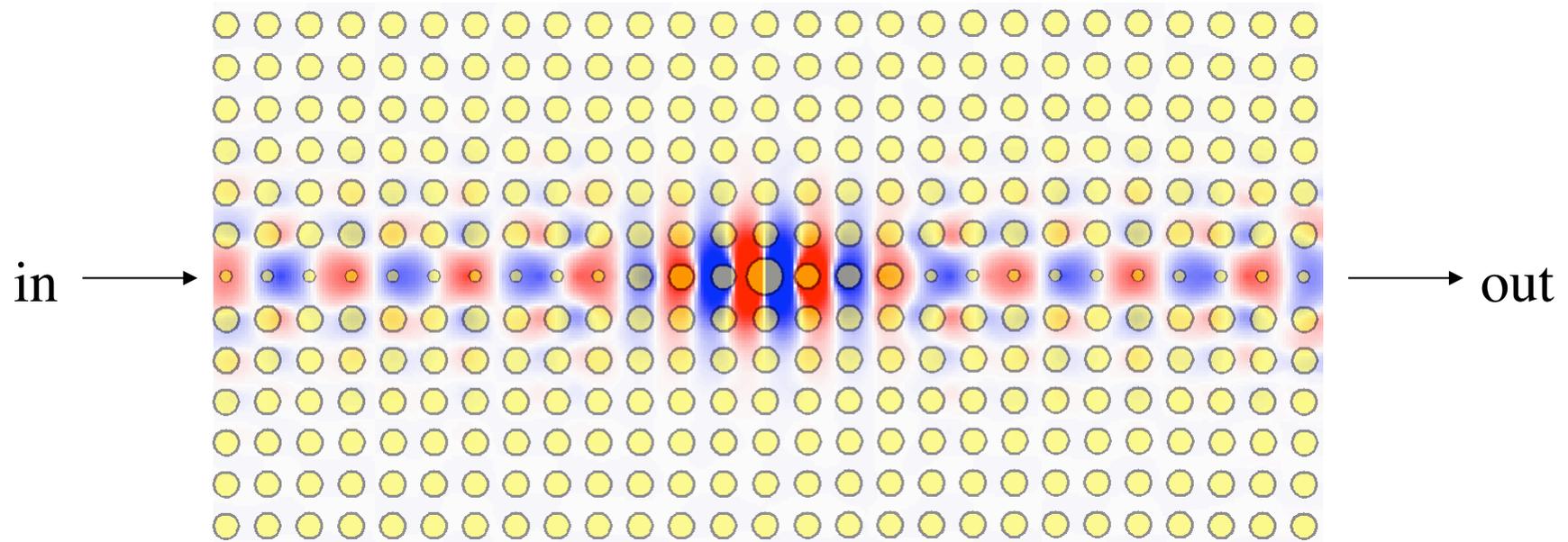
*That's not all!*

nonlinearities + microcavities

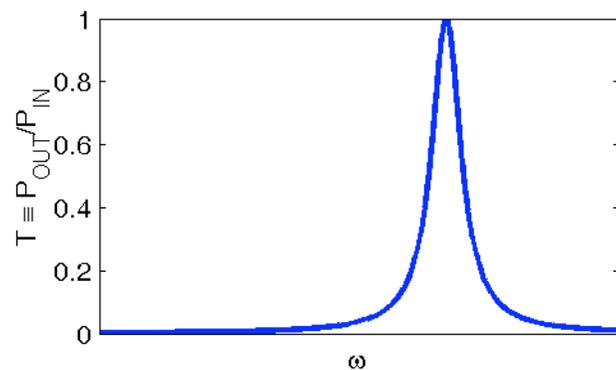
= *qualitatively* new phenomena

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

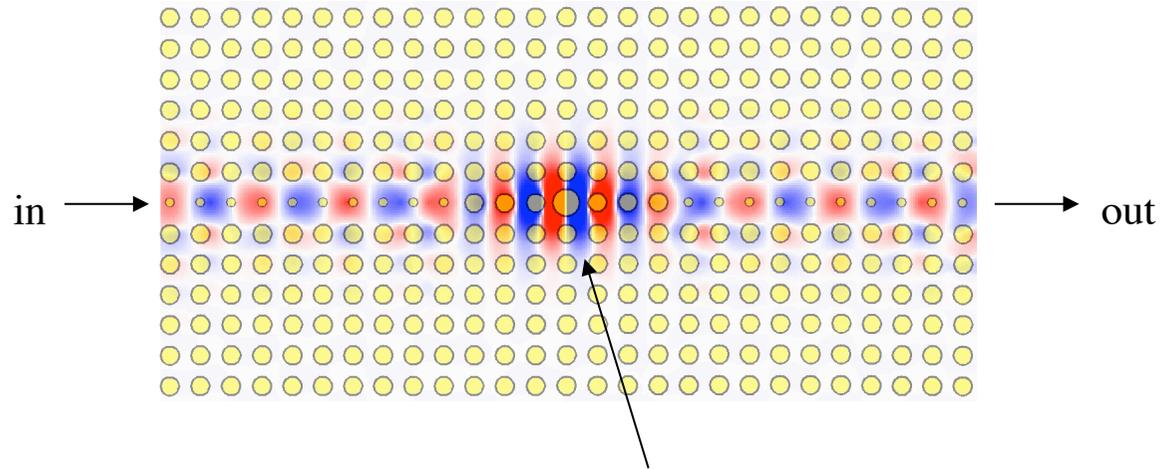
# A Simple Linear Filter



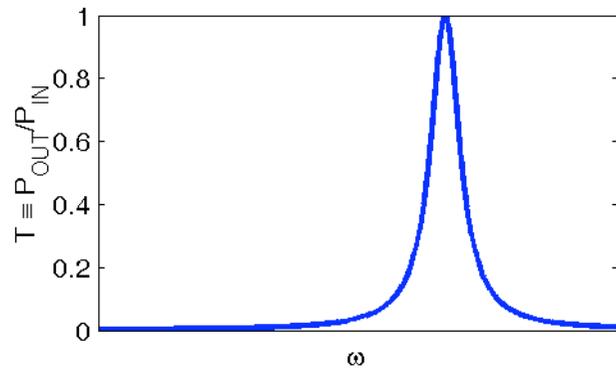
Linear response:  
Lorentzian Transmisson



# Filter + Kerr Nonlinearity?



Linear response:  
Lorentzian Transmisson



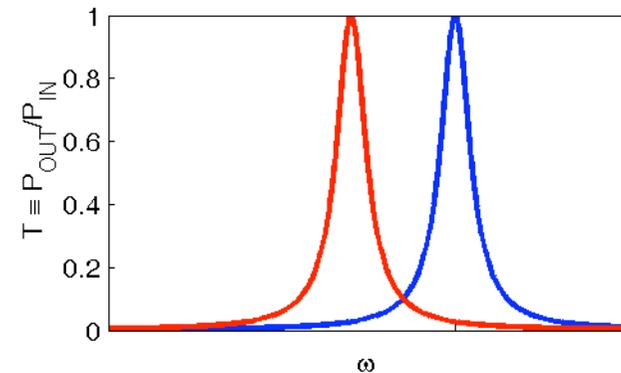
Kerr nonlinearity:

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

shifted peak?

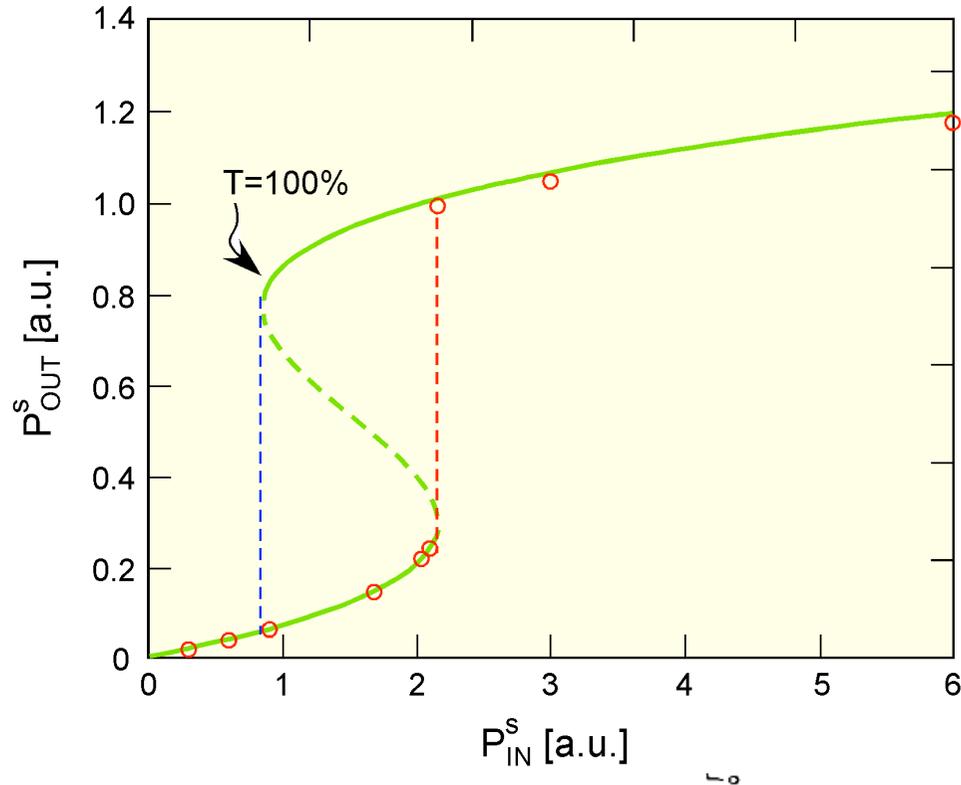


+ nonlinear  
index shift  
=  $\omega$  shift

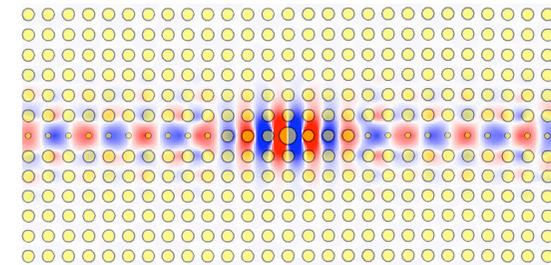


# Optical Bistability

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



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



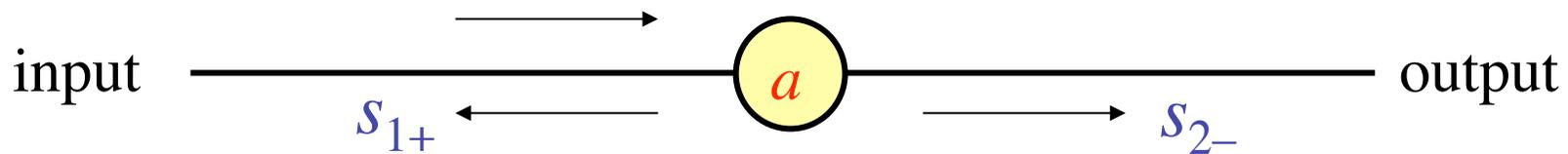
[ Soljagic *et al.*,  
*PRE Rapid. Comm.* **66**, 055601 (2002). ]

**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  $\omega_0$ , lifetime  $\tau$ ,

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

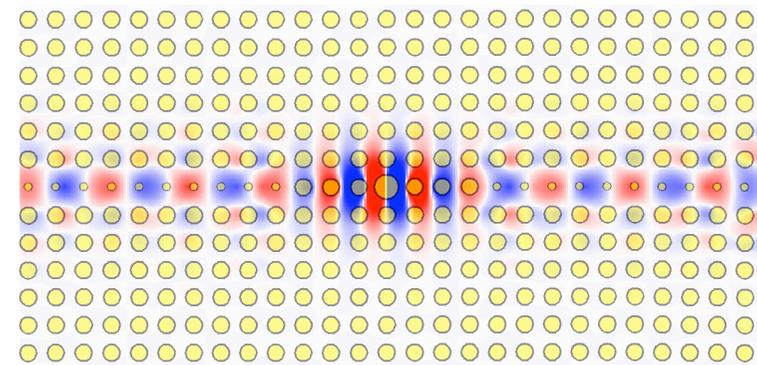
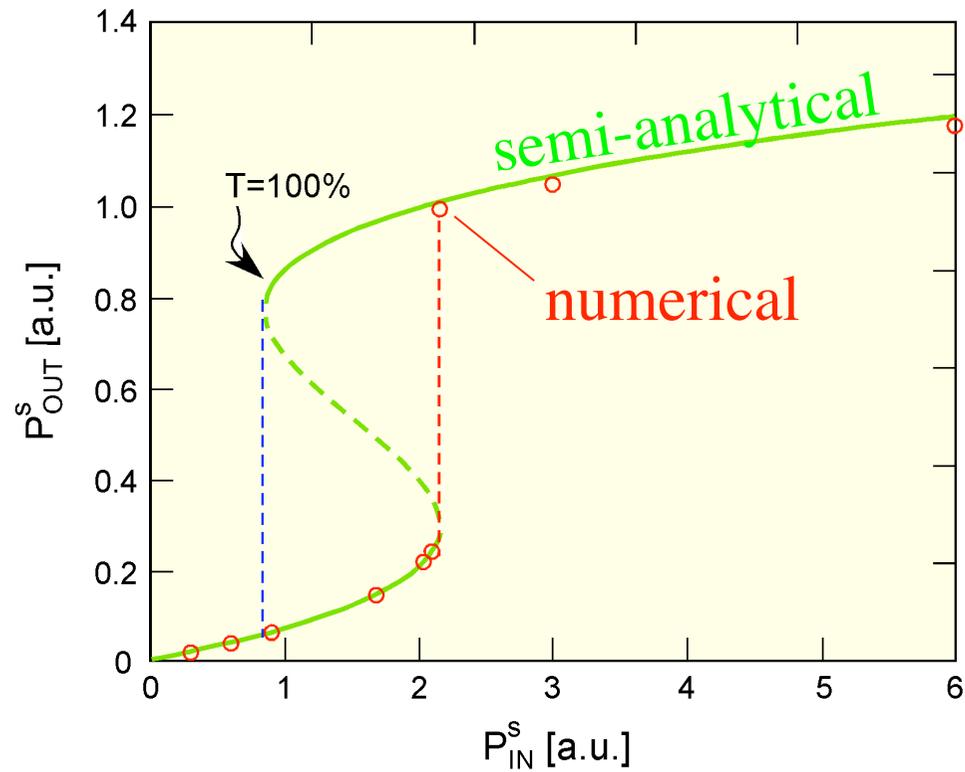
... evaluate  $\Delta\omega$  by 1st-order perturbation theory

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

$\Rightarrow$  all **relevant parameters** ( $\omega$ ,  $\tau$  or  $Q$ ,  $\alpha$ ) can be computed from the resonant mode of the **linear system**

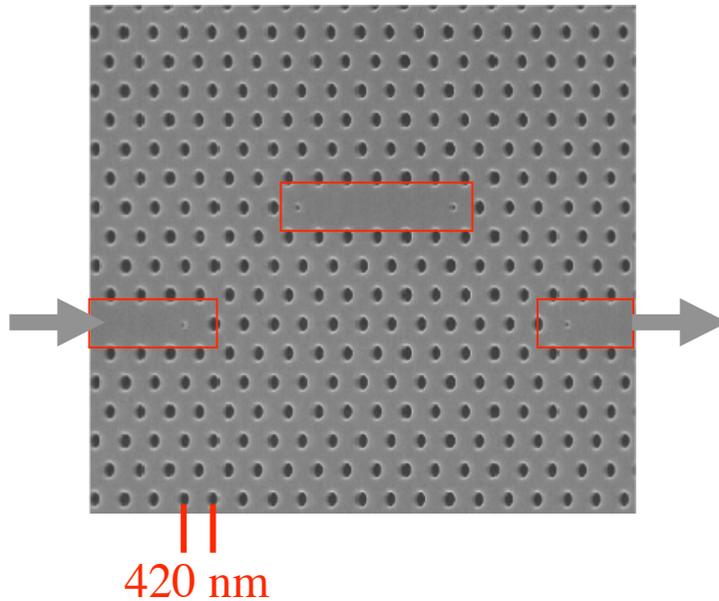
# Accuracy of Coupled-Mode Theory

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



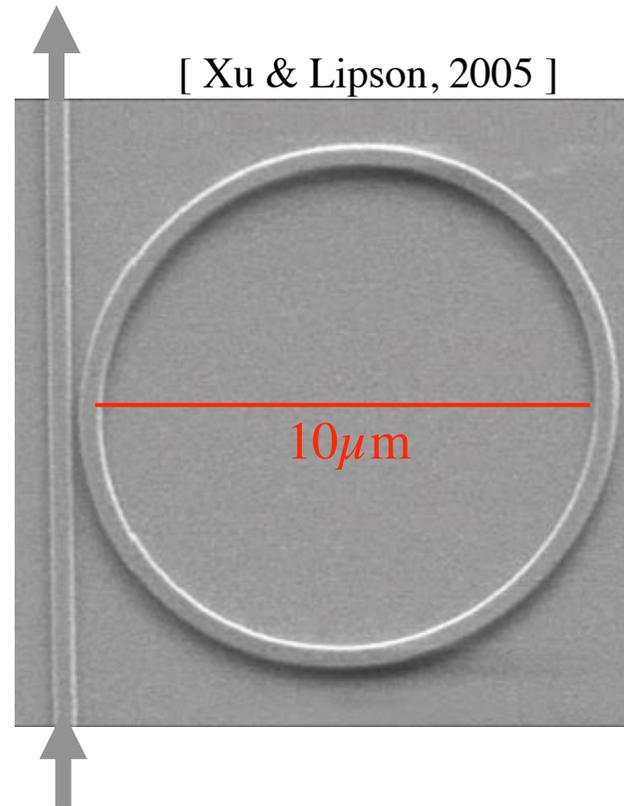
# Optical Bistability in Practice

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



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

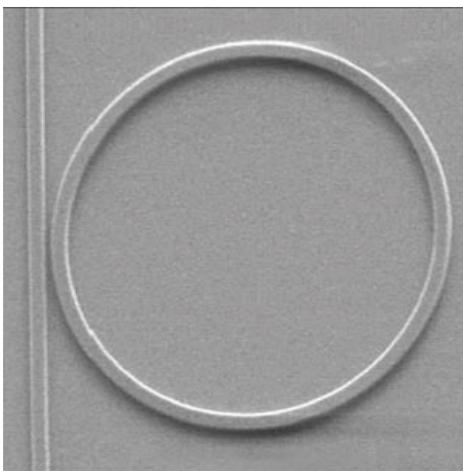
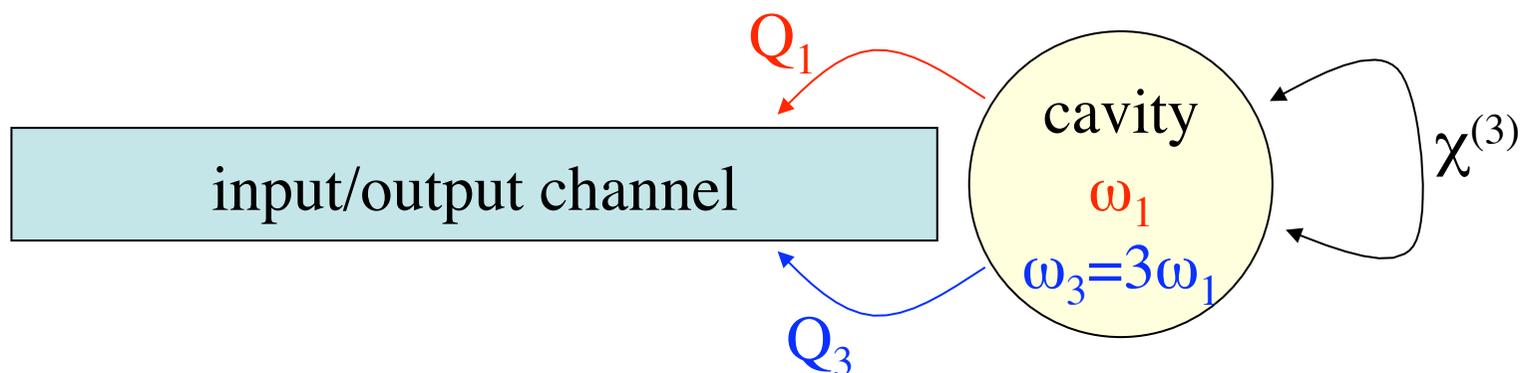
[ Xu & Lipson, 2005 ]



$Q \sim 10,000$   
 $V \sim 300$  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

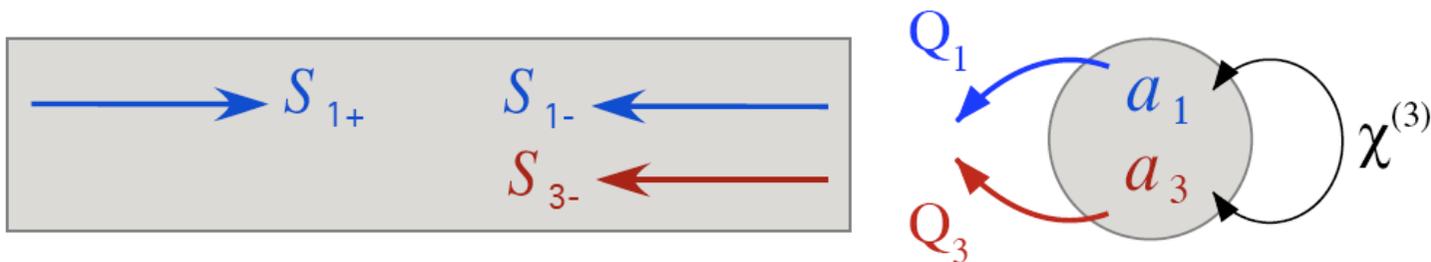
- must precisely tune  $\omega_3 / \omega_1$
- materials must be ok at  $\omega_1$  and  $3\omega_1$

*But ... what if we could do it?*

*... what are the consequences?*

# Coupled-mode Theory for THG

third harmonic generation

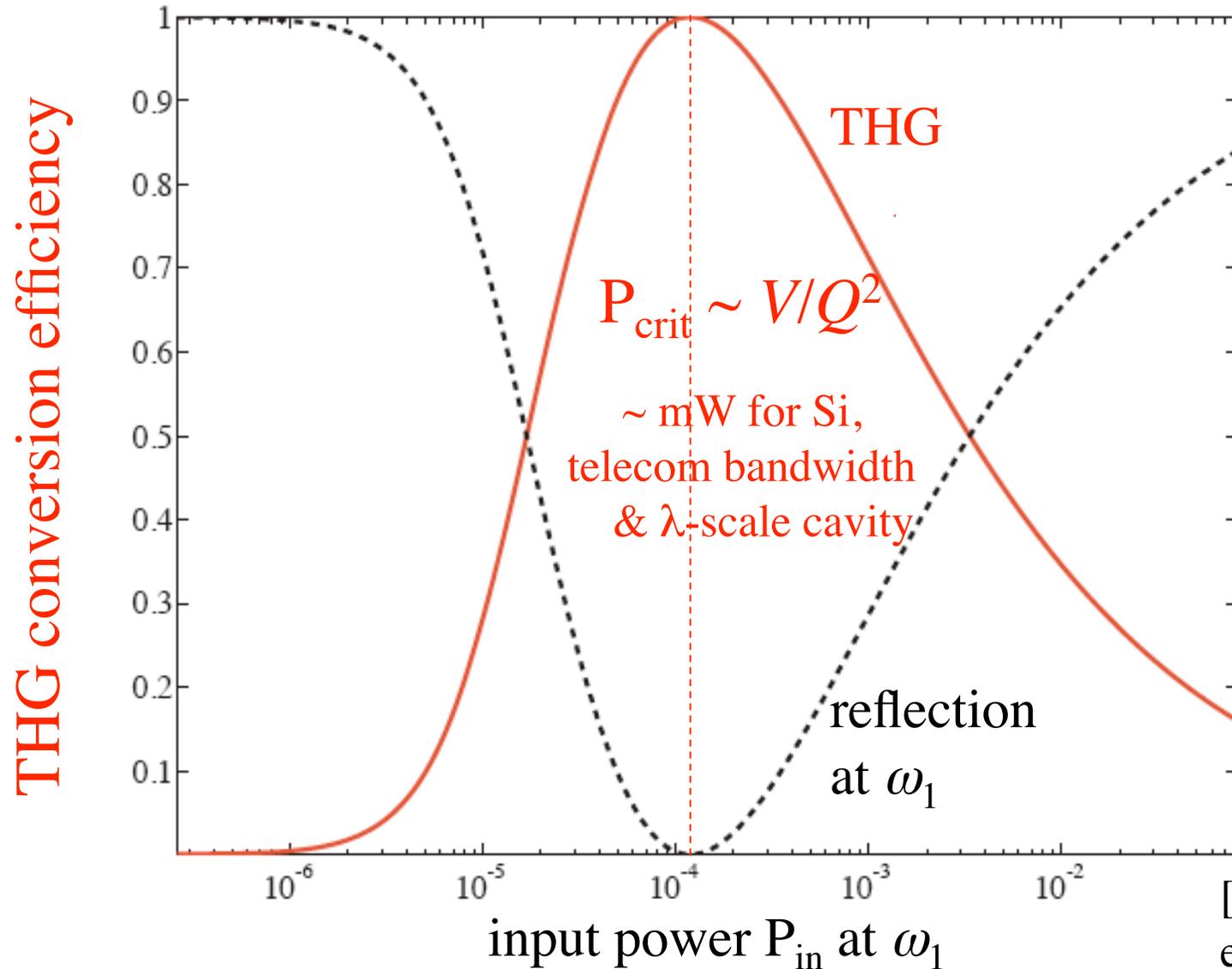


$$\begin{aligned} \frac{da_1}{dt} &= \left( \overset{\text{SPM}}{i\omega_1 (1 - \alpha_{11} |a_1|^2 - \alpha_{13} |a_3|^2)} - \frac{1}{\tau_1} \right) a_1 - \overset{\text{XPM}}{i\omega_1 \beta_1 (a_1^*)^2 a_3} + \overset{\text{down-conversion}}{\sqrt{\frac{2}{\tau_{s,1}}} s_+} \\ \frac{da_3}{dt} &=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

[ Rodriguez et al. (2007) ]

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

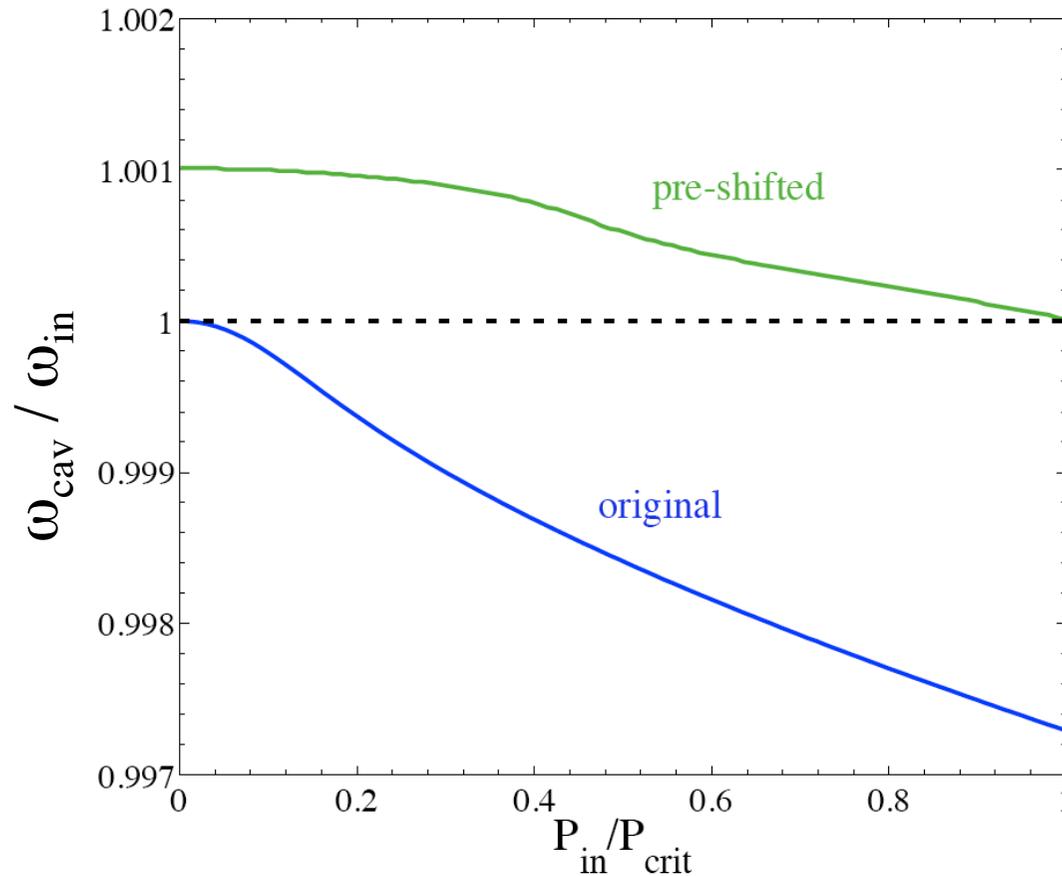
third-harmonic generation in doubly-resonant  $\chi^{(3)}$  (Kerr) cavity



[ 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?

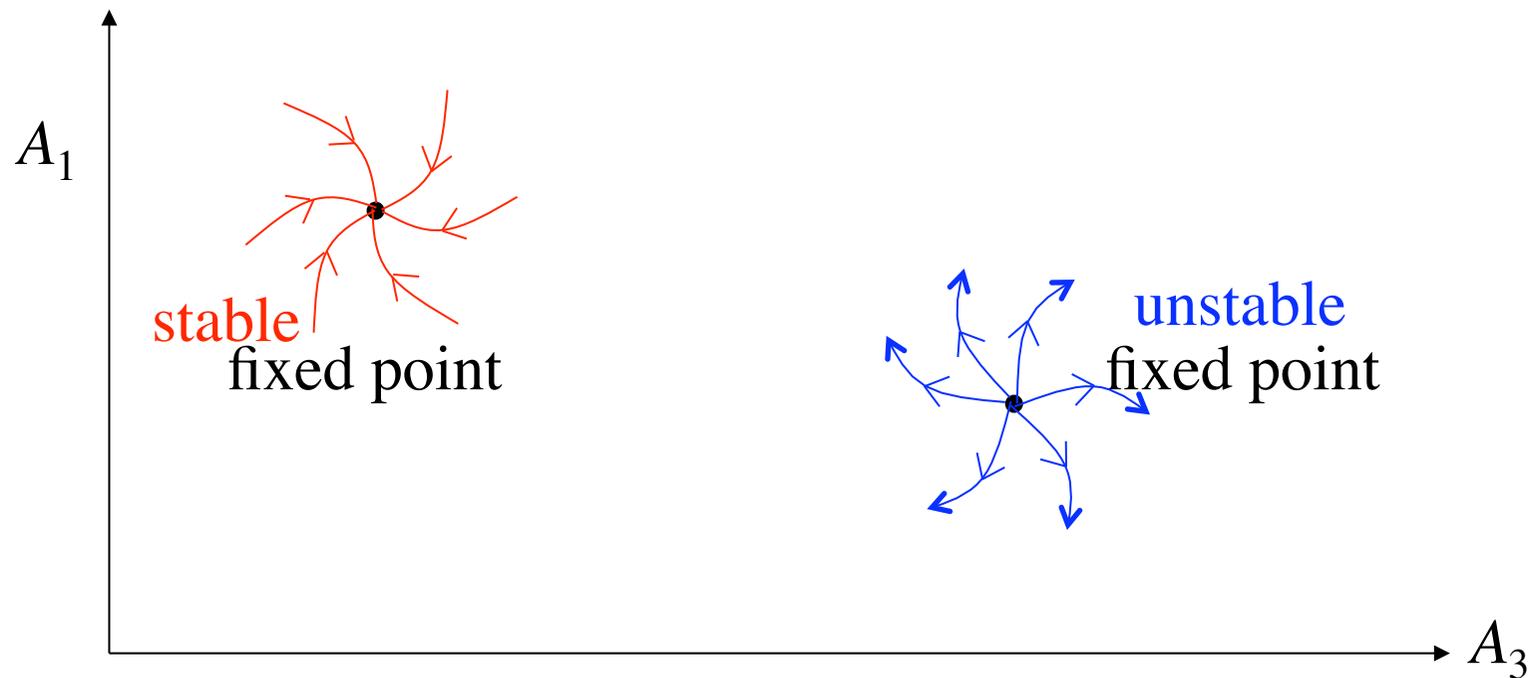
## *brief review*

Steady state-solution:  $a_1$  oscillating at  $\omega_1$ ,  $a_3$  at  $\omega_3$

— 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**



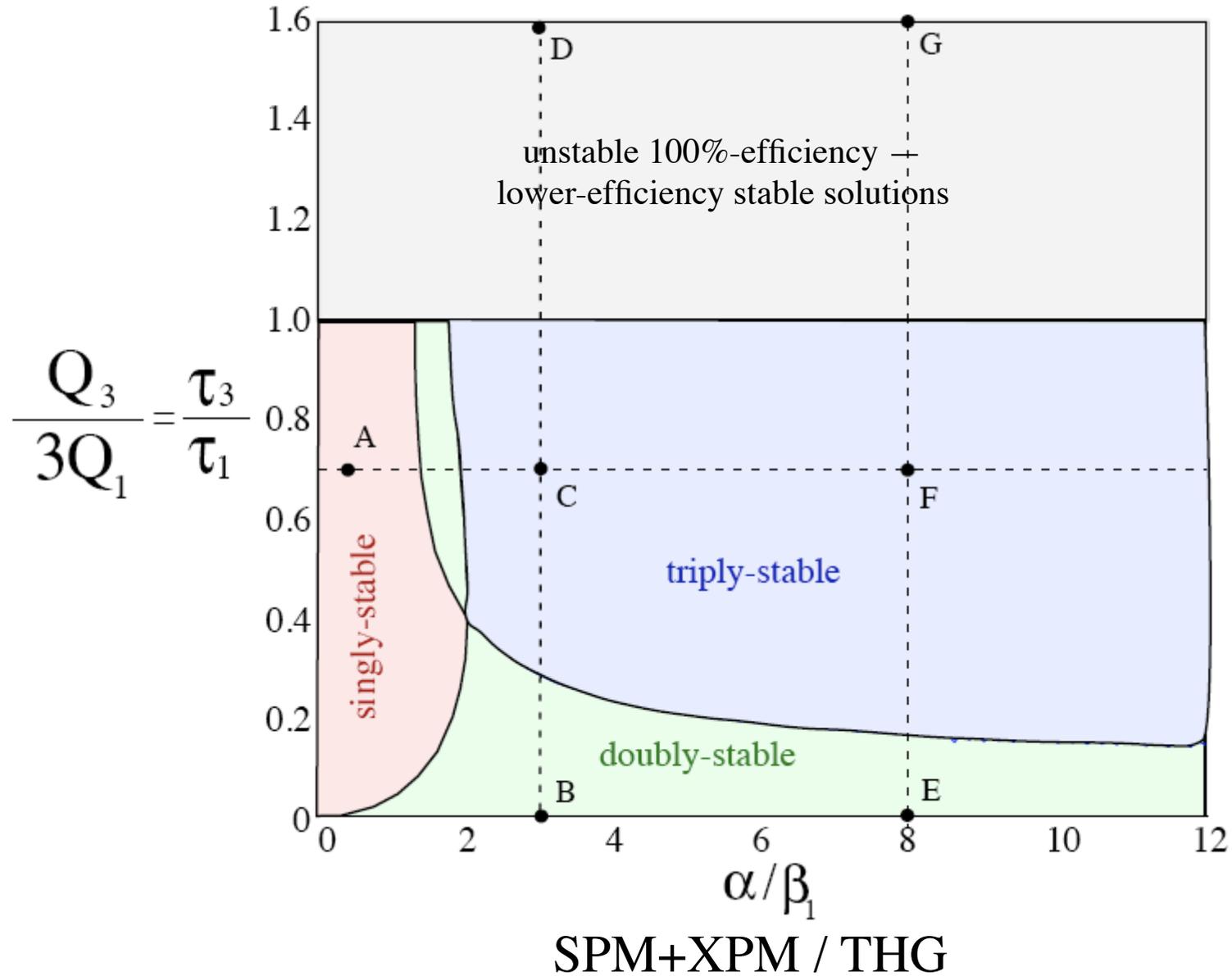
cartoon phase space ( $A_1, A_3$  are actually complex)

*for simplicity, assume SPM = XPM coefficients:*

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

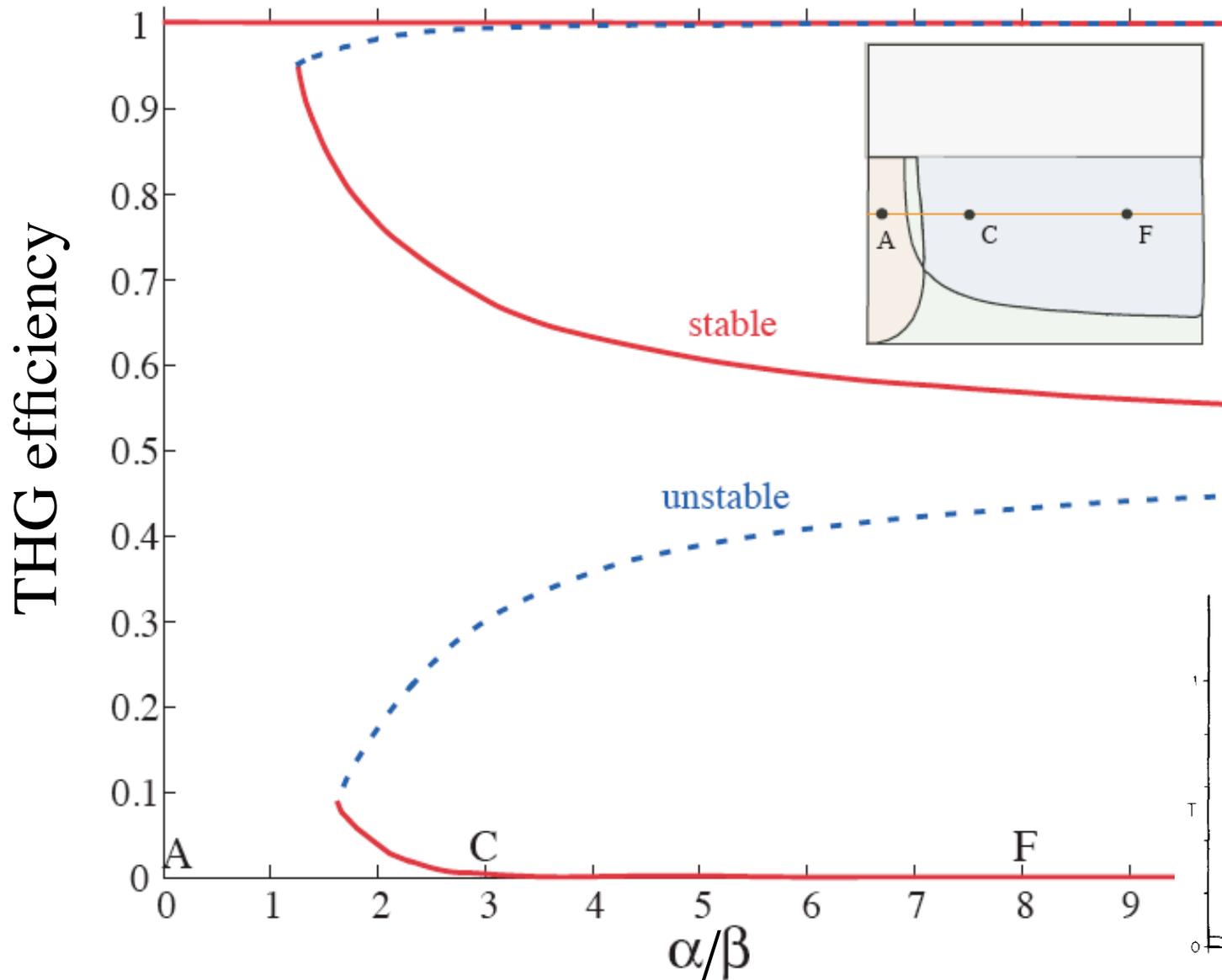
# THG Stability Phase Diagram

[ Hashemi et al (2008) ]

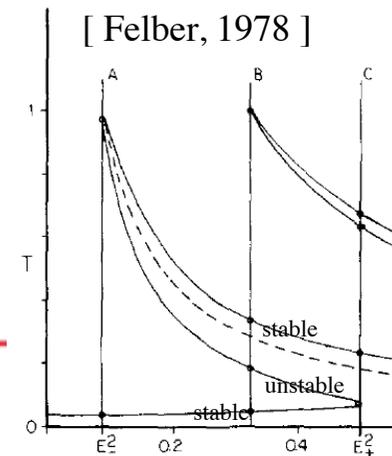


# Bifurcation vs. SPM/XPM

[ Hashemi et al (2008) ]



[ Felber, 1978 ]



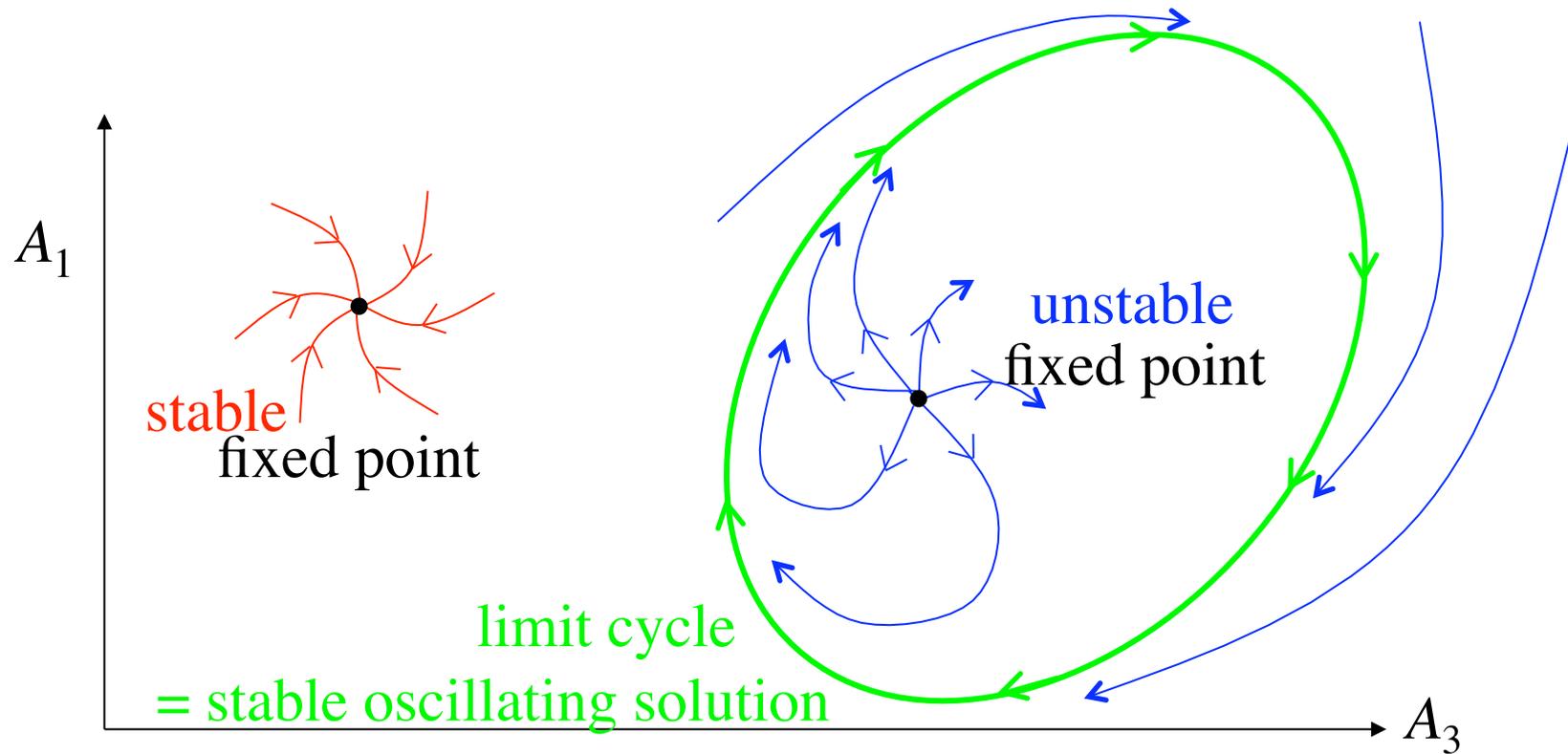
# Limit Cycles

Steady state-solution:  $a_1$  oscillating at  $\omega_1$ ,  $a_3$  at  $\omega_3$

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

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

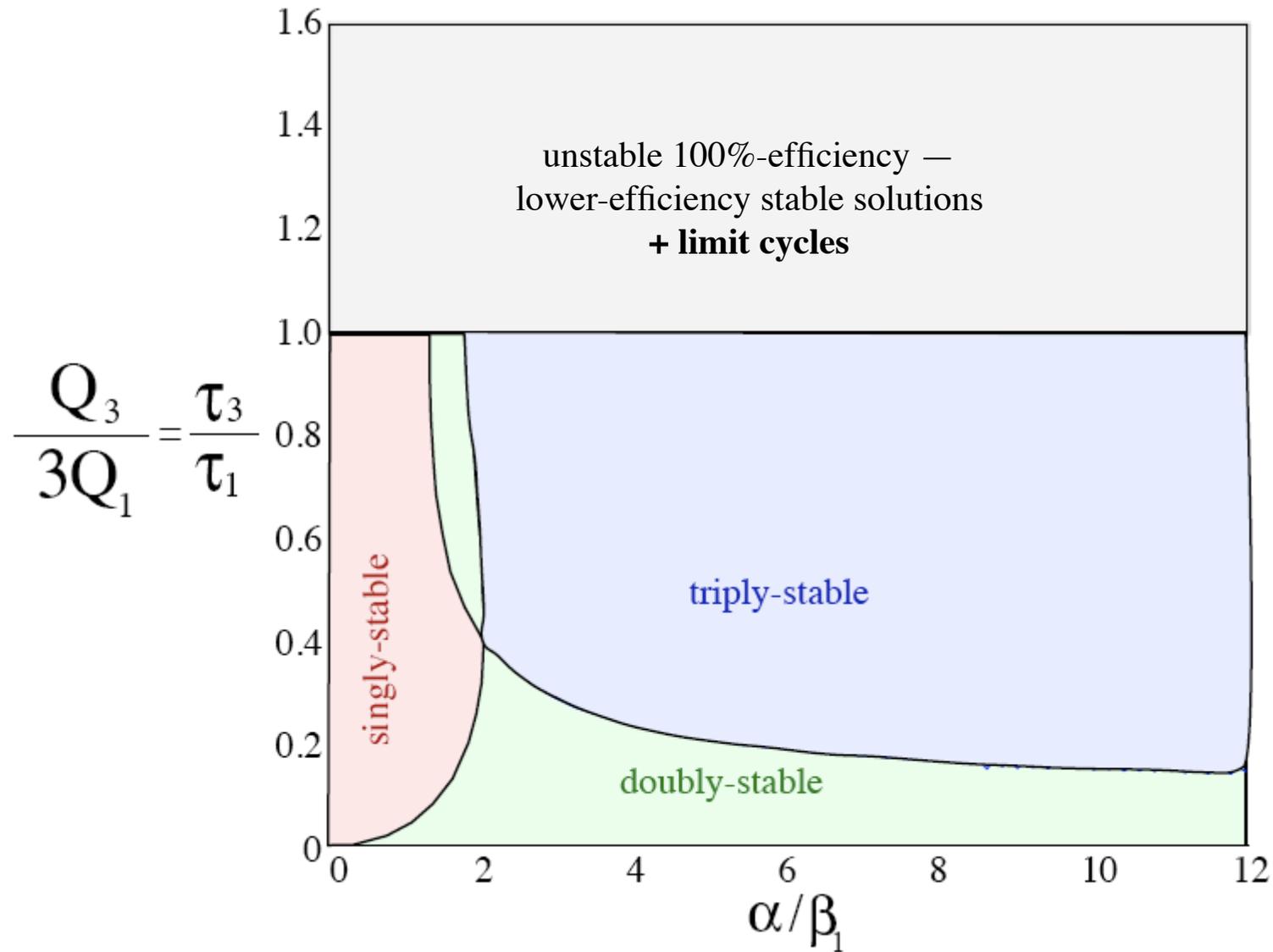
then steady state =  $A_1, A_3$  constant = **fixed-point**



cartoon phase space ( $A_1, A_3$  are actually complex)

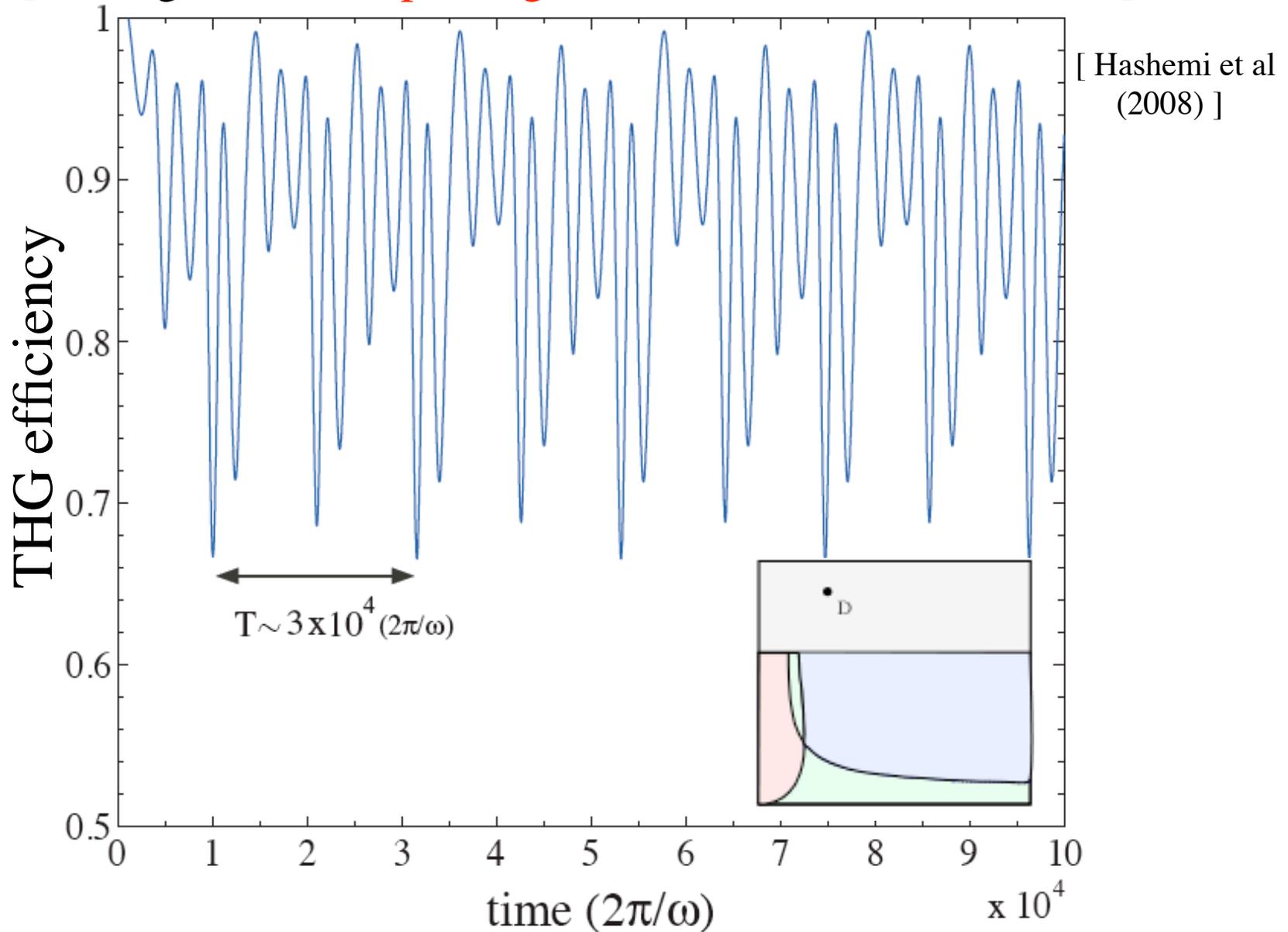
# Stability Phase Diagram

[ Hashemi et al (2008) ]



# An Optical Kerr-THG Oscillator

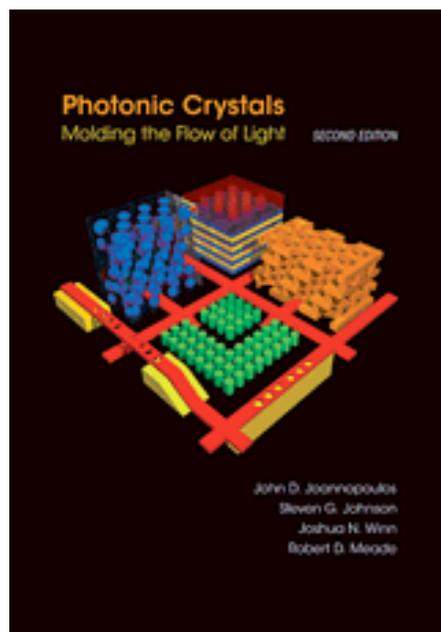
[ analogous to **self-pulsing** in SHG; Drummond (1980) ]



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>